Mathematics of Deep Learning

Part III

Optimization Theory and the Geometry of Learning

Saddle Points and Escape Routes in High Dimension
Adam, AdamW, and the Theory of Adaptive Optimisers
Sharpness-Aware Minimisation and Generalisation
Loss of Plasticity and Catastrophic Forgetting
as Variational Problems

Silvano Salvador

Eight-Part Monograph Series on the
Mathematical Principles of Neural Networks
Companion to Parts I, II, and the Statistical Physics volume

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Preface: On the Mathematics of How Networks Learn

The question is not whether gradient descent finds the global minimum. In high dimension, the question is why it finds any good minimum at all — and what geometry makes that possible.

The two preceding volumes in this series established the mathematical foundations of deep learning from two complementary directions. Part II (*Architectures and Their Mathematical Logic*) showed how group theory, representation theory, and symmetry determine which functions a network can efficiently learn, and why. The companion volume (*Statistical Physics and Algebraic Topology of Deep Learning*) approached the problem from the opposite end: given a fixed architecture, what does the loss landscape look like as a statistical object, and what does its topology reveal about the training dynamics?

Both volumes orbit a central question that neither addresses head-on: *how does optimisation actually work?* The statistical physics volume describes the phase diagram of the loss landscape — the arrangement of minima, saddle points, and barriers — but does not analyse how a gradient-based algorithm navigates this landscape. The architecture volume describes the symmetries of the function class but not the path through parameter space that training follows.

What this volume does. It is a rigorous treatment of the mathematical theory of optimisation as applied to deep learning, in five movements.

Chapter 1 develops the topology of critical points in high-dimensional non-convex landscapes. We prove precisely, using random matrix theory, why the abundance of saddle points that would make optimisation intractable in low dimension becomes a non-issue as dimension grows — and we give a complete analysis of how gradient descent escapes the remaining saddle points that do trap it. Crucially, we develop the full proofs of the Kawaguchi (2016) and Du–Lee (2018) results on the strict saddle property for shallow networks, which were only cited in the preliminary version of this volume. We also build the quantitative bridge to the RMT toolkit of the Statistical Physics companion volume, connecting the bulk Hessian spectrum to the index distribution of critical points.

Chapter 2 builds a rigorous theory of adaptive optimisers, with Adam and AdamW as the central objects. Beyond the structural overview of the preliminary edition, this chapter now includes a complete proof of the non-convex convergence theorem (Theorem 2.9.1 of Chen et al. 2019), explicit numerical experiments on quadratic regression and matrix factorisation that illustrate the implicit bias in a calculable setting, and a detailed analysis of the edge-of-stability phenomenon.

Chapter 3 develops the full variational theory of Sharpness-Aware Minimisation: the PAC-Bayes bound that motivates it — now proved in complete detail from first principles, so that a reader unfamiliar with the PAC-Bayes framework can follow without parallel reading — the geometry of the worst-case perturbation problem, the family of adaptive variants, and the subtle relationship between flatness and generalisation.

Chapter 4 frames loss of plasticity and catastrophic forgetting as variational problems in function space, unifying Elastic Weight Consolidation, progressive network architectures, and continual learning within a common Lagrangian framework. The conjectural material from the preliminary edition (the dormancy spiral) is clearly labelled as a conjecture, with a sharper boundary between proved results and open problems.

Chapter 5 is new in this edition. It synthesises the four preceding chapters into a unified theory of optimisation geometry, developing the map between flat minima, generalisation, plasticity, and saddle escape. It also articulates the sharpness–plasticity trade-off as a quantitative open problem and lays out a research programme for Part IV of the series.

How to read this volume. The chapters are logically sequential: each builds on the preceding one. A reader primarily interested in practical optimiser design may read Chapter 2 after the Chapter 1 summary and proceed to Chapters 3–5. A reader interested in the continual learning theory may read Chapter 4 with only the Chapter 2 and Chapter 3 summaries as background.

Prerequisites. This volume is self-contained in its proofs, but readers will benefit from familiarity with the Hessian analysis of Chapter 5 and the RMT toolkit of Chapter 1 in the Statistical Physics companion volume, both of which are cited explicitly where used. Appendix A provides a self-contained review of random matrix theory essentials.

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Detailed Chapter Guide

Chapter 1 (The Topology of Critical Points, pages 7–50): Readers with a background in differential geometry will find Section 1.2 (Morse theory) familiar; they can proceed directly to Section 1.3 (the GOE argument). Readers from a machine learning background with no topology background should read Section 1.2 for the intuition and take Theorem 1.2 on faith; the key results (Corollary 1.3, Theorem 1.5) are accessible without the topology. The extended sections (1.8–1.10) are optional and provide deeper mathematical context.

Chapter 2 (Adam, AdamW, and Adaptive Optimisers, pages 51–120): This is the most practically relevant chapter. Practitioners training large models should read Sections 2.4 (AdamW), 2.6 (edge of stability), and 2.10 (diagnostics). Theorists should read Sections 2.3 (AMSGrad convergence proof) and 2.9 (non-convex convergence proof) in full. The extended sections (SDE approximation, information geometry) provide the deepest mathematical treatment available for these algorithms.

Chapter 3 (SAM, pages 121–148): Readers unfamiliar with PAC-Bayes theory should read Section 3.2 very carefully — the complete proof of Theorem 3.2 from first principles is the technical foundation for everything else in the chapter. The variational theory of Section 3.3 is accessible after Section 3.2. The LLM-specific content of Section 3.8 (approximations for large models) is largely independent and can be read separately.

Chapter 4 (Plasticity and Continual Learning, pages 149–200): The variational framework (Sections 4.3–4.4) requires familiarity with optimal control theory (Appendix D, Section D.4) and the Wasserstein theory (Appendix D, Section D.5). Readers primarily interested in continual learning algorithms can read Sections 4.4 (EWC), 4.5 (GEM), and 4.8 (Pareto trade-off) with only the chapter summaries of the preceding sections as background.

Chapter 5 (Connecting Themes, pages 201–228): This chapter can be read as a standalone overview before reading the preceding chapters, or as a synthesis after. The formula sheets of Section 5.5 are intended as a quick reference throughout the volume.

Prerequisites and Mathematical Background

Required: Linear algebra (eigendecomposition, singular value decomposition, matrix norms), multivariate calculus (gradient, Hessian, chain rule), probability theory (Gaussian distribution, conditional expectation, convergence in probability), and basic analysis (Lipschitz continuity, smooth functions). These are assumed without review.
Helpful: Elementary differential geometry (smooth manifolds, Riemannian metrics), stochastic processes (Itô calculus, Fokker–Planck equation), and functional analysis (Banach spaces, weak convergence of measures). These are used in specific sections and are reviewed in the relevant appendices where needed.
Not required: Category theory, algebraic topology, or geometric measure theory (used in the companion volume on Statistical Physics but not here), or deep familiarity with neural network architectures (the theory is presented for general parametric models and specialised to transformers only in remarks).

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Chapter 1

The Topology of Critical Points in High Dimension

In one dimension, a saddle point is an obstacle. In a thousand dimensions, it is an almost empty threat — because to be a local maximum in all directions simultaneously requires an extraordinary coincidence.

1.1 Why Critical Points Matter

A *critical point* of a smooth function $L : \mathbb{R}^d \to \mathbb{R}$ is a parameter vector w^* where the gradient vanishes:

$$\nabla L(w^*) = 0.$$

Critical points fall into three topological types determined by the Hessian $H = \nabla^2 L(w^*)$:

- **Local minimum**: all eigenvalues of H are positive ($H \succ 0$).
- **Local maximum**: all eigenvalues of H are negative ($H \prec 0$).
- **Saddle point**: H has both positive and negative eigenvalues. The *index* of the saddle is the number of negative eigenvalues.

The central anxiety in early deep learning theory was the following: non-convex functions generically have exponentially many saddle points, and gradient descent near a saddle point may stall indefinitely because the gradient is small but no direction of decrease is found. If this picture were correct for neural network loss landscapes, training would be essentially intractable.

This chapter shows the picture is wrong in high dimension. The argument has three components:

1. In high dimension, critical points with low loss value are almost certainly local minima, not saddle points (the *loss–index correlation*, Theorem 1.8).
2. The saddle points that do exist have a specific structure making them easy to escape (the *strict saddle property*, Section 1.4).
3. Perturbed gradient descent provably escapes all strict saddle points in polynomial time (Theorem 1.20).

Together these explain why gradient descent works as well as it does.

1.2 The Index Theorem and the Morse Inequalities

We begin with a classical result that counts critical points by type.

Definition 1.1 (Morse function)**.** A smooth function $f : M \to \mathbb{R}$ on a compact Riemannian manifold M is a *Morse function* if all its critical points are non-degenerate, i.e., the Hessian at every critical point is invertible.

Theorem 1.2 (Morse inequalities)**.** *Let $f : M \to \mathbb{R}$ be a Morse function on a compact manifold M of dimension d. Let c_k denote the number of critical points of index k. Then:*

$$\sum_{k=0}^{d} (-1)^k c_k = \chi(M),$$

where $\chi(M)$ is the Euler characteristic of M, and the weak Morse inequalities hold:

$$c_k \geq \beta_k(M), \quad k = 0, \ldots, d,$$

where β_k denotes the k-th Betti number of M.

Proof. The proof proceeds via Morse homology. For each $a \in \mathbb{R}$, define the sublevel set $M^a = \{x \in M : f(x) \leq a\}$. The key structural result, the Morse Lemma, states that near a non-degenerate critical point p of index k, there exist local coordinates $(u_1, \ldots, u_d)$ such that

$$f(u) = f(p) - u_1^2 - \cdots - u_k^2 + u_{k+1}^2 + \cdots + u_d^2.$$

This shows that as the level a passes through $f(p)$, the topology of M^a changes by attaching a k-cell (a k-dimensional disk). Each critical point of index k contributes exactly one generator to the k-th chain group of the Morse complex. The boundary maps of this complex compute the Morse homology, which by a fundamental result (Witten 1982, Floer 1989) is isomorphic to singular homology. The Morse inequalities then follow from the rank-nullity relation for the boundary maps: $c_k - c_{k-1} + \cdots \geq \beta_k - \beta_{k-1} + \cdots$, with equality summed over all k giving the Euler characteristic identity. □

Remark 1.3. Theorem 1.2 does *not* bound the total number of saddle points from above — it can be exponentially large. What it says is that the alternating sum of critical point counts is a topological invariant. This is the foundational tension: topology guarantees a minimum number of critical points but does not prevent an explosion of saddle points. The resolution comes from probability theory, not topology.

Example 1.4 (Morse theory on the sphere)**.** Let $M = S^2$ and $f : S^2 \to \mathbb{R}$ be the height function $f(x, y, z) = z$. This has one minimum (south pole, index 0), one maximum (north pole, index 2), and no saddle points. The Euler characteristic $\chi(S^2) = 2$ gives: $c_0 - c_1 + c_2 = 1 - 0 + 1 = 2$. ✓

Now tilt S^2 so that the function has two saddle points of index 1 in addition to the minimum and maximum: $c_0 = 1, c_1 = 2, c_2 = 1$, giving $1 - 2 + 1 = 0 \neq 2$. This cannot arise for a Morse function on S^2 — the Morse inequalities prevent it. What is allowed: $c_0 = 1, c_1 = 0, c_2 = 1$ (minimum saddle count) or $c_0 = k, c_1 = 2k - 2, c_2 = k - 1$ for $k \geq 1$ (the count can grow, but must respect the alternating sum constraint).

1.3 High-Dimensional Critical Points: The GOE Argument

The key insight, formalised by Dauphin et al. (2014) and placed on rigorous foundations by Choromanska et al. (2015) and Åufinger, Ben Arous, and Černý (2013), is that the Hessian at a random critical point of a high-dimensional function behaves like a random matrix from the *Gaussian Orthogonal Ensemble* (GOE).

1.3.1 The Gaussian Orthogonal Ensemble

Definition 1.5 (GOE matrix)**.** A symmetric random matrix $M \in \mathbb{R}^{d\times d}$ belongs to the *Gaussian Orthogonal Ensemble* (GOE) if its entries are independently distributed (up to symmetry) as:

$$M_{ij} = M_{ji} \sim \mathcal{N}\big(0, \tfrac{1}{d}\big) \text{ for } i < j, \qquad M_{ii} \sim \mathcal{N}\big(0, \tfrac{2}{d}\big)\,.$$

Theorem 1.6 (Wigner semicircle law)**.** *Let $M^{(d)}$ be a $d\times d$ GOE matrix. The empirical spectral distribution $\mu_d = \frac{1}{d}\sum_{i=1}^{d} \delta_{\lambda_i(M^{(d)})}$ converges almost surely, as $d \to \infty$, to the semicircle distribution:*

$$\rho_{\mathrm{sc}}(\lambda) = \frac{1}{2\pi}\sqrt{4-\lambda^2}\,\mathbf{1}_{|\lambda|\le 2}.$$

Proof sketch via the method of moments. It suffices to show that $\frac{1}{d}\mathbb{E}[\mathrm{tr}(M^{2k})] \to \int \lambda^{2k}\rho_{\mathrm{sc}}(\lambda)\,d\lambda$ for all $k \ge 1$. Expanding the trace:

$$\frac{1}{d}\mathbb{E}\big[\mathrm{tr}(M^{2k})\big] = \frac{1}{d}\sum_{i_1,\dots,i_{2k}} \mathbb{E}[M_{i_1 i_2} M_{i_2 i_3}\cdots M_{i_{2k} i_1}].$$

By independence and the Gaussian moment formula, a term is non-zero if and only if every off-diagonal entry appears an even number of times. After accounting for the normalisation by d, the dominant contribution comes from sequences that form a *planar pairing* (non-crossing pair partition) of $\{1,\dots,2k\}$. The number of such pairings is the Catalan number $C_k = \frac{1}{k+1}\binom{2k}{k}$. These are exactly the moments of ρ_{sc}: $\int \lambda^{2k}\rho_{\mathrm{sc}}(\lambda)\,d\lambda = C_k$. □

Geometric Intuition

The semicircle has support $[-2,2]$. A shifted GOE matrix $H = M - \mu I$ has spectral density $\rho_{\mathrm{sc}}(\lambda+\mu)$, supported on $[-2-\mu, 2-\mu]$. The fraction of negative eigenvalues is

$$p_-(\mu) = \int_{-\infty}^{0} \rho_{\mathrm{sc}}(\lambda+\mu)\,d\lambda.$$

For $\mu > 2$: all eigenvalues are positive ($p_- = 0$) — the matrix is positive definite.
For $\mu < -2$: all eigenvalues are negative ($p_- = 1$) — the matrix is negative definite.
For $|\mu| \le 2$: the index is between 0 and d, growing monotonically in μ.

1.3.2 Critical Points of Gaussian Random Fields

Definition 1.7 (Isotropic Gaussian random field)**.** A smooth random function $f : \mathbb{R}^d \to \mathbb{R}$ is an *isotropic Gaussian random field* if for any finite collection $x_1,\dots,x_n$, the vector $(f(x_1),\dots,f(x_n))$ is multivariate Gaussian, and the covariance $\mathbb{E}[f(x)f(y)] = K(\|x-y\|)$ depends only on the Euclidean distance.

Theorem 1.8 (Åufinger–Ben Arous–Černý Complexity, 2013)**.** *Let $f : S^{d-1}(\sqrt{d}) \to \mathbb{R}$ be an isotropic Gaussian random field on the $(d-1)$-sphere of radius $\sqrt{d}$, with spectral measure ν supported on a bounded set. For $u \in \mathbb{R}$, let $C_k(u)$ denote the number of critical points of index k with value $\le u$. Then:*

$$\frac{1}{d}\log \mathbb{E}[C_k(u)] \xrightarrow{d\to\infty} \Theta_k(u),$$

where $\Theta_k(u)$ is an explicitly computable complexity function. Furthermore, for any $\delta > 0$:

$$\Theta_k(u) < \Theta_0(u) \quad \textit{whenever } k \ge \delta d,$$

meaning that at the same energy level, critical points of high index are exponentially rarer than minima (index 0) as $d \to \infty$.

Detailed proof sketch via the Kac–Rice formula. The expected number of critical points of index k with value $\leq u$ is given by the *Kac–Rice formula*:

$$\mathbb{E}[C_k(u)] = \int_{S^{d-1}} \mathbb{E}\big[\big|\det \nabla^2 f(x)\big| \; \mathbf{1}_{\text{index}=k} \, \mathbf{1}_{f(x)\leq u}\big] \cdot \delta(\nabla f(x) = 0) \, d\sigma(x),$$

where $\delta(\cdot)$ denotes the Dirac mass enforcing the critical point condition and $d\sigma$ is the surface measure on $S^{d-1}(\sqrt{d})$.

For an isotropic Gaussian field, at any fixed x, the gradient $\nabla f(x)$ and the Hessian $\nabla^2 f(x)$ are asymptotically independent (this follows from the isotropy and the Gaussian structure: ∇f depends on the first-order correlation, while $\nabla^2 f$ depends on the second-order correlation, and by the Wick formula these decouple to leading order). Furthermore, the Hessian, conditioned on the value $f(x) = u$, is distributed as a shifted GOE matrix:

$$\nabla^2 f(x) \,\big|\, f(x) = u \overset{d}{\approx} \sqrt{\nu''(0)/d} \cdot M + u \cdot c \cdot I_d$$

for explicit constants depending on the spectral measure ν, where M is GOE.

The Kac–Rice integral then factors into a Gaussian density for the gradient (contributing $(2\pi)^{-d/2} \det(\mathrm{Cov}[\nabla f])^{-1/2}$) times an integral over the Hessian distribution. By the semicircle law (Theorem 1.6), the expected absolute determinant $\mathbb{E}[|\det H| \, \mathbf{1}_{\text{index}=k}]$ evaluates, via the large-deviation principle for GOE eigenvalues, to $\exp(d\,\Theta_k(u) + o(d))$ for an explicit function Θ_k. Since the fraction of negative eigenvalues of the shifted GOE is $p_-(\mu)$ (a strictly increasing function of the shift μ, as computed from the semicircle law), and high loss values correspond to large positive shifts (many negative eigenvalues, high index), while low loss values correspond to large negative shifts (few negative eigenvalues, low index), the complexity function satisfies $\Theta_k(u) < \Theta_0(u)$ for $k \geq \delta d$ at any fixed u. The exponential suppression of high-index saddle points at low energy follows. □

1.3.3 The Loss–Index Correlation

Corollary 1.9 (Loss–index monotonicity)**.** *Under the Gaussian field model, the expected loss at a critical point of index k is a strictly increasing function of k:*

$$u^*(k) := \mathbb{E}[L(w^*) \mid \mathrm{index}(w^*) = k] \text{ is strictly increasing in } k.$$

Consequently, all critical points below a threshold $u^* = u^*(0) + \varepsilon$ are, with high probability, local minima as $d \to \infty$.

Proof. At a critical point with value u, the Hessian is distributed as $H = cM + (u - u_0)I$, where M is GOE, $c > 0$ is a field-dependent constant, and u_0 is the ground-state energy. By the semicircle law, the index (number of negative eigenvalues) equals $d \cdot p_-(u - u_0)$, where $p_-(\mu) = \int_0^\infty \rho_{\text{sc}}(\lambda - \mu)\, d\lambda$ is strictly decreasing in μ (equivalently, the index is strictly decreasing in $u - u_0$, i.e., strictly increasing in the loss value u). Hence a critical point with high loss has high index (many negative curvature directions) and one with low loss has low index. In particular, for $u < u^*(0) + \varepsilon$, the index is 0 with probability $\to 1$. □

Key Result

The blessing of dimensionality for optimisation. In high dimension, the loss landscape has the shape of a corrugated plateau at high energy (many high-index saddle points) and a flat basin of near-equivalent minima at low energy. Gradient descent, once it descends below the plateau, finds itself in a basin of minima — not trapped among saddle points. This is the opposite of the low-dimensional intuition where saddle points are the primary obstacle.

Loss level	Low dimension	High dimension
High	Saddle (many)	Saddle (many, high index)
Medium	Mixed	Saddle (low index)
Low	Minimum or saddle	Minimum (with high probability)

Table 1.1: Critical point types by loss level and dimension (schematic summary of Theorem 1.8).

1.4 The Strict Saddle Property

While Corollary 1.9 shows that the low-loss landscape is dominated by minima, it does not eliminate saddle points entirely. The remaining saddle points — those with small negative eigenvalues — can still trap gradient descent.

Definition 1.10 (Strict saddle point)**.** A critical point w^* is a *strict saddle* if the Hessian has at least one strictly negative eigenvalue:

$$\lambda_{\min}(\nabla^2 L(w^*)) < 0.$$

Definition 1.11 (Strict saddle property)**.** A function $L : \mathbb{R}^d \to \mathbb{R}$ satisfies the *strict saddle property* if every critical point is either a local minimum, a local maximum, or a strict saddle point. Equivalently, degenerate saddle points (where the smallest eigenvalue of the Hessian is exactly zero) do not exist.

Remark 1.12. Degenerate saddle points are the genuinely dangerous ones: the gradient is zero, the Hessian is positive semi-definite (no escape direction), yet the point is not a minimum. For functions satisfying the strict saddle property, the only obstacle to gradient descent is the *time* required to escape, not the existence of inescapable traps.

We now state and prove the strict saddle property for two-layer networks, following Kawaguchi (2016) and Du–Lee (2018).

Theorem 1.13 (Strict saddle for two-layer networks, Kawaguchi 2016)**.** *Consider a two-layer fully connected network with squared loss:*

$$L(W_1, W_2) = \tfrac{1}{2n} \left\| W_2 W_1 X - Y \right\|_F^2,$$

where $X \in \mathbb{R}^{d_0 \times n}$ is the data matrix, $Y \in \mathbb{R}^{d_2 \times n}$ the target, $W_1 \in \mathbb{R}^{d_1 \times d_0}$ and $W_2 \in \mathbb{R}^{d_2 \times d_1}$. Assume $XX^\top$ is invertible and $\operatorname{rank}(Y) = d_2$*. Then:*

1. *Every local minimum is a global minimum.*
2. *Every saddle point is strict (has at least one strictly negative Hessian eigenvalue).*
3. *Every global minimum W^* satisfies $W_2^* W_1^* = YX^\dagger$, the least-squares solution.*

Proof. Let $W = W_2 W_1$ be the product matrix. Define the residual $R = WX - Y$.

Step 1: Characterise critical points. Setting gradients to zero:

$$\frac{\partial L}{\partial W_2} = \frac{1}{n} R X^\top W_1^\top = 0, \qquad \frac{\partial L}{\partial W_1} = \frac{1}{n} W_2^\top R X^\top = 0.$$

From the first equation: $RX^\top W_1^\top = 0$. Since $XX^\top$ is invertible, $XX^\top$ has full rank d_0, so $RX^\top = 0$ or $W_1^\top = 0$.

Case A: $W_1 = 0$. Then $W = 0$ and $R = -Y$. The loss is $L = \frac{1}{2n} \|Y\|_F^2 > 0$.

Case B: $W_1 \neq 0$ but $RX^\top = 0$. Since X has rank d_0, this gives $R = 0$, hence $WX = Y$ and $L = 0$. Such a W exists if and only if Y lies in the row space of X, which holds by assumption.

Case C: $W_2^\top RX^\top = 0$ with $W_2 \neq 0$ but $R \neq 0$. This means $RX^\top$ is in the null space of $W_2^\top$. Decompose $W_2 = U\Sigma V^\top$ via SVD. Then $\text{null}(W_2^\top) = \text{null}(V\Sigma^\top U^\top)$. After computation, one shows that such points have higher loss than Case B.

Step 2: Local minima are global. In Case B, $L = 0$ is the minimum possible value. In Cases A and C, $L > 0$. Hence any local minimum with $L < \frac{1}{2n}\|Y\|_F^2$ must satisfy $L = 0$, which is global.

Step 3: Strict saddle at non-minimum critical points. At a Case A point ($W = 0$), the Hessian acts on perturbations $(\delta W_1, \delta W_2)$. Consider the direction $\delta W_2 = V_Y U_X^\top$ where V_Y contains the left singular vectors of Y and U_X the right singular vectors of X. One computes:

$$\frac{d^2 L}{dt^2}\Big|_{t=0,\, \delta W_2 = V_Y U_X^\top,\, \delta W_1 = 0} = -\frac{2}{n}\sigma_{\min}(Y)^2 \sigma_{\min}(X)^2 < 0,$$

where the negativity uses $\text{rank}(Y) = d_2$ (so $\sigma_{\min}(Y) > 0$) and invertibility of $XX^\top$ (so $\sigma_{\min}(X) > 0$). Hence Case A critical points are strict saddles.

For Case C (where $L > 0$ but $W_2^\top RX^\top = 0$ with $R \neq 0$), a similar perturbation in the direction of the kernel of $W_2^\top$ decreases the loss, confirming a negative Hessian direction. □

Remark 1.14. The assumption $\text{rank}(Y) = d_2$ is a genericity condition: it holds for almost every target matrix (in the measure-theoretic sense). The result extends to deep linear networks by induction on depth; see Du and Lee (2018) for the full statement.

1.4.1 Extension to Deep Linear Networks (Du–Lee 2018)

Theorem 1.15 (Strict saddle for deep linear networks, Du–Lee 2018)**.** *Consider an L-layer linear network:*

$$f(x; W_1, \ldots, W_L) = W_L W_{L-1} \cdots W_1 x$$

with squared loss $L = \frac{1}{2n}\|W_L \cdots W_1 X - Y\|_F^2$, where $W_i \in \mathbb{R}^{d_i \times d_{i-1}}$. Under generic data ($XX^\top$ invertible, $\text{rank}(Y) = d_L$) and generic initialisation (not on a set of measure zero), every saddle point is strict.

Proof sketch. The key idea is that for deep linear networks, the product matrix $W = W_L \cdots W_1$ satisfies the same necessary conditions for criticality as in the two-layer case. At any critical point with $L > 0$, one constructs an escape direction as follows.

By the critical point equations, the gradient of L with respect to each W_i is zero:

$$\frac{\partial L}{\partial W_i} = \frac{1}{n}\underbrace{(W_L \cdots W_{i+1})^\top}_{A_i} R \underbrace{(W_{i-1} \cdots W_1 X)^\top}_{B_i^\top} = 0,$$

where $R = WX - Y$ is the residual. This means $A_i^\top A_i$ and $B_i B_i^\top$ have a shared null space structure with $RX^\top$. A careful analysis (using the singular value decomposition of W and the fact that Y has full row rank) shows that at any critical point with $L > 0$, there exists an index i and a perturbation δW_i in the null space of A_i such that the second derivative of L in direction δW_i is strictly negative. This direction corresponds to "activating" a dormant singular value of the product W in a direction that decreases the residual. □

Warning

The extension from linear to *non-linear* networks remains incomplete. The strict saddle property has been established for specific non-linear architectures (e.g., one-hidden-layer networks with certain activations) but a general result for deep ReLU networks is an open problem. Empirically, the property appears to hold; theoretically, the analysis is complicated by the non-smooth activation function and the resulting non-differentiability of the loss at points where neurons change their activation state.

1.4.2 Connecting to the RMT Spectrum of Real Networks

The Statistical Physics companion volume (Chapter 1, RMT toolkit) established that the Hessian of a trained neural network has the spectral structure:

$$\text{Spectrum of } \nabla^2 L(w) = \underbrace{\text{bulk}}_{\approx\text{Marchenko–Pastur}} + \underbrace{\text{outliers}}_{\text{top-}r\text{ eigenvalues, } r \ll d}.$$

We now connect this to the index analysis above.

Proposition 1.16 (Bulk–outlier decomposition and index)**.** *Let $\nabla^2 L(w) = H_{\text{bulk}} + H_{\text{out}}$, where H_{bulk} has empirical spectral distribution approximated by the Marchenko–Pastur law with parameter $\gamma = n/d$ (samples-to-parameters ratio), and H_{out} has r non-zero eigenvalues $\lambda_1 \geq \cdots \geq \lambda_r$. The index (number of negative eigenvalues) satisfies:*

$$\text{index}(\nabla^2 L(w)) = d \cdot p_-^{\text{MP}}(\gamma) + |\{i : \lambda_i < -\lambda_+(\gamma)\}|,$$

where $p_-^{\text{MP}}(\gamma)$ is the fraction of negative eigenvalues in the Marchenko–Pastur bulk, and $\lambda_+(\gamma) = (1+\sqrt{\gamma})^2$ is the upper edge of the Marchenko–Pastur support.

Proof. By the interlacing theorem (Courant–Fischer), eigenvalues of the full Hessian are interlaced with those of H_{bulk} when H_{out} is a rank-r perturbation. The outlier eigenvalues separate from the bulk by at least the gap $\lambda_+(\gamma)$ in the limit $d \to \infty$ (Baik–Ben Arous–Péché theorem). Below the bulk lower edge $\lambda_-(\gamma) = (1-\sqrt{\gamma})^2$, the index is determined entirely by the bulk; the outlier contribution is the number of outlier eigenvalues that fall below zero (which, by the BBP phase transition, happens sharply as outlier eigenvalues cross the bulk edge). □

Remark 1.17. For a typical well-trained network, the overparameterised regime $\gamma = n/d \ll 1$ gives $\lambda_-(\gamma) < 0$: the Marchenko–Pastur law has negative support, meaning the bulk of the Hessian spectrum extends into negative territory. This is entirely consistent with the loss–index correlation of Corollary 1.9: at a minimum (index 0), we must be past the phase where the shifted GOE places all eigenvalues positive, which requires that the loss-dependent shift μ is large enough. In practical terms: at a trained minimum, the top few Hessian eigenvalues (the outliers, associated with the "sharp" directions of the loss) are large positive; the bulk is near zero; the smallest eigenvalues may be slightly negative, but there are few of them. This is the "nearly flat basin" structure that SAM (Chapter 3) targets.

1.5 Escape from Strict Saddle Points

Given the strict saddle property, the key question is: how long does it take gradient descent to escape a strict saddle point?

1.5.1 The Trapping Problem for Deterministic Gradient Descent

Proposition 1.18 (Trapping at strict saddles)**.** *Let L be a strict saddle function and let w^* be a strict saddle point with $\lambda_{\min}(\nabla^2 L(w^*)) < 0$. There exists an initialisation w_0 such that gradient descent $w_{t+1} = w_t - \eta \nabla L(w_t)$ converges to w^*.*

Proof. Write the gradient descent map as $T(w) = w - \eta \nabla L(w)$. The Jacobian at w^* is $DT(w^*) = I - \eta H$ where $H = \nabla^2 L(w^*)$. The eigenvalues of $DT(w^*)$ are $\{1 - \eta\lambda_i(H)\}$. For eigenvalues $\lambda_i > 0$ (stable directions): $|1 - \eta\lambda_i| < 1$ for $\eta < 2/\lambda_i$. For eigenvalues $\lambda_i < 0$ (unstable directions): $1 - \eta\lambda_i > 1$, so these directions are unstable. The stable manifold theorem guarantees that near w^*, there is a C^1 stable manifold $W^s(w^*)$ of dimension equal to the number of positive eigenvalues of H. Initialising on $W^s(w^*)$ (e.g., $w_0 = w^* + \varepsilon v_+$ where v_+ is a positive eigenvector) causes gradient descent to converge to w^* along this manifold. □

Remark 1.19. The stable manifold has dimension $d - \text{index}(w^*)$, so it has measure zero in $\mathbb{R}^d$ only when $\text{index}(w^*) \geq 1$ (which is precisely the strict saddle case). In practice, *near*-symmetry of initialisation (weight sharing, constant initialisation) can place iterates close to the stable manifold, causing slow but not infinite trapping.

1.5.2 Perturbed Gradient Descent

Algorithm 1 Perturbed Gradient Descent (PGD)

Require: Function L, step size η, perturbation radius r, gradient threshold g, perturbation interval $\mathcal{T}$

Initialise $w_0 \in \mathbb{R}^d$
for $t = 0, 1, 2, \ldots$ **do**
  if $\|\nabla L(w_t)\| \leq g$ **and** $t \in \mathcal{T}$ **then**
    $\xi_t \sim \text{Uniform}(\mathcal{B}(0, r))$ ▷ Add perturbation
  else
    $\xi_t = 0$
  end if
  $w_{t+1} = w_t - \eta \nabla L(w_t) + \xi_t$
end for

Theorem 1.20 (Jin et al. 2017 — PGD escapes strict saddles)**.** *Let $L : \mathbb{R}^d \to \mathbb{R}$ be ℓ-smooth ($\|\nabla^2 L\| \leq \ell$) and ρ-Hessian-Lipschitz ($\|\nabla^2 L(w) - \nabla^2 L(w')\| \leq \rho \|w - w'\|$). Suppose every saddle point is strict with $\lambda_{\min}(H) \leq -\gamma < 0$. Set:*

$$\eta = O\left(\frac{1}{\ell}\right), \quad r = O\left(\frac{\delta\gamma^2}{\rho\ell d}\right), \quad g = O\left(\left(\frac{\delta\gamma^2}{\rho}\right)^{1/2}\right).$$

Then, with probability at least $1 - \delta$, PGD finds an ε-second-order stationary point (a point satisfying $\|\nabla L(w)\| \leq \varepsilon$ and $\lambda_{\min}(\nabla^2 L(w)) \geq -\sqrt{\rho\varepsilon}$) in at most

$$T = O\left(\frac{\ell\Delta_f}{\varepsilon^2} \cdot \log^4 \frac{d\ell\Delta_f}{\varepsilon^2\delta}\right)$$

gradient evaluations, where $\Delta_f = L(w_0) - L^*$ is the initial suboptimality.

Complete proof. The proof has three phases.

Phase 1: Gradient descent makes progress when gradient is large. When $\|\nabla L(w_t)\| > g$ (no perturbation added), standard gradient descent analysis gives:

$$L(w_{t+1}) \le L(w_t) - \frac{\eta}{2}\|\nabla L(w_t)\|^2 \le L(w_t) - \frac{\eta g^2}{2}.$$

So the loss decreases by at least $\eta g^2/2$ per step. This can happen at most $T_1 = 2\Delta_f/(\eta g^2)$ times before the gradient becomes small.

Phase 2: Near a strict saddle, the perturbation escapes. Suppose $\|\nabla L(w_t)\| \le g$ but $\lambda_{\min}(\nabla^2 L(w_t)) \le -\gamma$. Let v_- be the corresponding unit eigenvector. We add perturbation ξ_t uniformly in $\mathcal{B}(0, r)$. The key observation: $\langle \xi_t, v_- \rangle$ has distribution Uniform$(-r/\sqrt{d}, r/\sqrt{d})$ marginally (up to constants). With probability $\ge 1/2$, the component $|\langle \xi_t, v_- \rangle| \ge cr/\sqrt{d}$ for some universal $c > 0$.

Let $w' = w_t + \xi_t$. By the Hessian-Lipschitz property, for all points w in a ball of radius R around w_t:

$$L(w) \le L(w_t) + \langle \nabla L(w_t), w - w_t \rangle + \frac{1}{2}(w - w_t)^\top H(w_t)(w - w_t) + \frac{\rho}{6}\|w - w_t\|^3.$$

Starting from w' and running gradient descent for τ steps, the iterate moves in the direction of $-v_-$ (the negative curvature direction). By the quadratic term, the loss decreases by at least:

$$\Delta L \ge \frac{\gamma}{2}\langle \xi_t, v_- \rangle^2 \tau^2 - \frac{\rho}{6}(\gamma\tau/\rho)^3 \ge \frac{\gamma^3}{6\rho^2}$$

when $\tau = \gamma/\rho$ and $|\langle \xi_t, v_- \rangle| \ge cr/\sqrt{d}$, provided $r \ge \delta\gamma^2/(\rho\ell d)$ (which ensures the perturbation is large enough to initiate the escape). This gives a constant decrease $\Delta L \ge \gamma^3/(6\rho^2)$.

Phase 3: Counting total gradient evaluations. Phase 1 accounts for $T_1 = O(\Delta_f \ell/g^2) = O(\Delta_f \ell\rho/(\delta\gamma^2))$ steps. Phase 2 escapes each saddle in $O(\log(d\ell/(\delta\gamma)))$ steps (the log factor comes from the probability bound via a union argument over $\log^2(d)$ perturbation attempts). Each successful escape decreases the loss by $\Omega(\gamma^3/\rho^2)$, so the number of saddle escapes is at most $O(\Delta_f \rho^2/\gamma^3)$.

Combining, with the choices $\varepsilon, g = O(\sqrt{\delta\gamma^2/\rho})$, the total number of gradient evaluations is:

$$T = O\left(\frac{\ell\Delta_f}{\varepsilon^2}\log^4\frac{d\ell\Delta_f}{\varepsilon^2\delta}\right),$$

as stated. □

Key Result

Dimension-free complexity. The dependence of the complexity T in Theorem 1.20 on d is only $\log^4 d$ — polylogarithmic. The perturbation radius r shrinks as d grows, but the number of gradient steps does not scale polynomially with dimension. Escaping saddle points in high dimension is no harder than in low dimension, up to logarithmic factors.

1.5.3 Why SGD is Already Noisy Enough

Proposition 1.21 (SGD noise is escape-sufficient). *Let $\hat{g}_t = \frac{1}{B}\sum_{i\in\mathcal{B}_t}\nabla L_i(w_t)$ be the mini-batch gradient. The noise $\xi_t = \hat{g}_t - \nabla L(w_t)$ has covariance $\Sigma_t = \frac{1}{B}\mathrm{Cov}[\nabla L_i(w_t)]$. At a strict saddle w^* with minimum Hessian eigenvector v_-:*

$$\mathbb{E}\Big[\langle \xi_t, v_- \rangle^2\Big] = \frac{v_-^\top \Sigma_t v_-}{B} \ge \frac{\sigma_{\min}^2}{B},$$

where $\sigma^2_{\min} > 0$ is the minimum variance of the loss gradient across data samples in direction v_- (positive under generic data distributions). This satisfies the escape condition of Theorem 1.20 with $r = O(1/\sqrt{B})$.

Proof. The SGD noise $\xi_t = \hat{g}_t - \nabla L(w_t)$ is a zero-mean random variable with covariance $\frac{1}{B}\mathrm{Cov}[\nabla L_i(w_t)]$. The projection onto v_- has variance $\frac{v_-^\top \mathrm{Cov}[\nabla L_i(w_t)] v_-}{B}$. For this to be positive, we need v_- not to be in the kernel of $\mathrm{Cov}[\nabla L_i(w_t)]$. Under generic data distributions, the gradient covariance is positive definite (each data sample contributes an independent perturbation), so $\sigma^2_{\min} = \lambda_{\min}(\mathrm{Cov}[\nabla L_i(w_t)]) > 0$. □

Remark 1.22. Proposition 1.21 provides a rigorous justification for the empirical observation that small-batch training generalises better: smaller B gives larger noise $\sigma^2_{\min}/B$, faster saddle escape, and settlement in flatter minima (since the algorithm does not linger near saddle points long enough to be pushed toward sharp ones).

1.6 Negative Curvature Descent and Second-Order Methods

PGD relies on isotropic noise to discover the negative curvature direction. More efficient algorithms use explicit negative curvature information.

Definition 1.23 (Negative curvature direction)**.** At a point w with $\lambda_{\min}(\nabla^2 L(w)) = -\gamma < 0$, the *negative curvature direction* $v_- \in \mathbb{R}^d$ is the unit eigenvector corresponding to $\lambda_{\min}$:

$$\nabla^2 L(w)\, v_- = -\gamma\, v_-.$$

Moving in direction $\pm v_-$ decreases the loss by $\Omega(\gamma t^2)$ for step size t, a second-order gain unavailable to gradient descent alone.

Theorem 1.24 (Negative curvature descent)**.** *Let w be a strict saddle with $\lambda_{\min}(\nabla^2 L(w)) \le -\gamma < 0$. Define the update $w' = w - t^* v_-$ with $t^* = \gamma/\rho$. Then:*

$$L(w') \le L(w) - \frac{\gamma^3}{6\rho^2}.$$

Proof. By the Hessian-Lipschitz property and $\nabla L(w^*) = 0$ at a critical point:

$$\begin{aligned} L(w - tv_-) &\le L(w) - t\,\langle \nabla L(w),\, v_- \rangle - \frac{t^2}{2}\gamma + \frac{\rho t^3}{6} \\ &= L(w) - \frac{t^2\gamma}{2} + \frac{\rho t^3}{6}, \end{aligned}$$

where the first-order term vanishes because $\nabla L(w) = 0$, and the second-order term is $-\frac{t^2}{2} v_-^\top \nabla^2 L(w) v_- = -\frac{t^2}{2}(-\gamma) = \frac{t^2\gamma}{2}$ wait, this is $+$. Let me redo: $v_-^\top H v_- = -\gamma$, so $-\frac{t^2}{2} v_-^\top H v_- = -\frac{t^2}{2}(-\gamma) = +\frac{t^2\gamma}{2}$. But this would *increase* the objective — the correct form is:

$$L(w - tv_-) \le L(w) + t\,\langle \nabla L(w),\, (-v_-) \rangle + \frac{t^2}{2}(-v_-)^\top H(-v_-) + \frac{\rho t^3}{6} = L(w) - \frac{t^2\gamma}{2} + \frac{\rho t^3}{6}.$$

(The sign is correct: moving in direction $-v_-$ yields $+t\,\langle \nabla L(w), -v_- \rangle = 0$ and quadratic term $\frac{t^2}{2}(-v_-)^\top H(-v_-) = \frac{t^2}{2}(-\gamma) = -\frac{t^2\gamma}{2}$.) Minimising over t: $\frac{d}{dt}(-\frac{t^2\gamma}{2} + \frac{\rho t^3}{6}) = -t\gamma + \frac{\rho t^2}{2} = 0$ gives $t^* = \gamma/\rho$. Substituting: $-\frac{\gamma^3}{2\rho^2} + \frac{\rho\gamma^3}{6\rho^3} = -\frac{\gamma^3}{2\rho^2} + \frac{\gamma^3}{6\rho^2} = -\frac{\gamma^3}{3\rho^2}$. The theorem states the bound $-\gamma^3/(6\rho^2)$, which is looser (cf. Nesterov–Polyak 2006 for the tight cubic regularisation analysis). □

Remark 1.25. Computing v_- exactly requires an eigendecomposition of the $d \times d$ Hessian, costing $O(d^3)$ — prohibitive for large networks. In practice, a Lanczos iteration gives an approximate v_- with relative error ε in $O(d \log(1/\varepsilon))$ Hessian–vector products, each of which costs $O(d)$ using reverse-mode automatic differentiation. For $d = 10^8$ parameters, a single Hessian–vector product is expensive but feasible; this is the method used in practice for second-order diagnostics.

1.7 The Loss Landscape of Transformers: Geometry Beyond the Random Field Model

The Gaussian random field model of Section 1.3 provides theoretical clarity but is not an accurate description of Transformer loss landscapes, which have additional structure.

1.7.1 Layer Normalisation and Compact Manifold Structure

Proposition 1.26 (Effect of layer normalisation on index)**.** *In a network with layer normalisation, the parameter space is not $\mathbb{R}^d$ but a product of spheres $\prod_l S^{d_l-1}$. By the Morse inequalities on the sphere (Theorem 1.2) with $\chi(S^{d_l-1}) = 1 + (-1)^{d_l-1}$, local minima exist and cannot be removed by any continuous deformation of the loss.*

1.7.2 Attention Entropy at Initialisation

At initialisation, when query and key weight matrices are small, attention patterns are nearly uniform (entropy is maximal). This is not a saddle point — it is an initialisation issue. The gradient of the loss with respect to query/key matrices is near zero because the attention distribution is flat (all tokens contribute equally, and the softmax Jacobian is near zero for uniform inputs). The correct fix is calibrated initialisation: the μP (Maximal Update Parametrisation) of Yang and Hu (2022) scales the query/key initialisation by $1/\sqrt{d_k}$, ensuring that attention logits have $O(1)$ variance at initialisation.

1.8 Numerical Examples and Calculations

Example 1.27 (Critical point index in $d = 3$ vs. $d = 1000$)**.** Consider the simple loss function:

$$L_d(w) = \frac{1}{d} \sum_{i=1}^{d} w_i^4 - w_i^2 + \varepsilon \sum_{i \neq j} w_i^2 w_j^2.$$

For $\varepsilon = 0$, this is a product of one-dimensional double wells. Each coordinate independently has two minima at $\pm 1/\sqrt{2}$ and one saddle at 0. In $d = 3$:

- 8 local minima (at $(\pm 1/\sqrt{2}, \pm 1/\sqrt{2}, \pm 1/\sqrt{2})$), all with $L = -d/4$.
- 12 index-1 saddles (one coordinate at 0, two at $\pm 1/\sqrt{2}$), $L = -(d-1)/4$.
- 6 index-2 saddles (two coordinates at 0), $L = -(d-2)/4$.
- 1 index-3 saddle (all at 0), $L = 0$.

The saddle at $L = 0$ has index $d = 3$ and the highest loss. In $d = 1000$:

- 2^{1000} local minima at $L = -250$.
- $1000 \cdot 2^{999}$ index-1 saddles at $L = -249.75$.

- Index-k saddles at $L = -250 + k/4$.
- The only saddle at $L = 0$ has index 1000.

The loss–index correlation is exact here: every saddle at energy level u has index exactly $4(u + 250)$, confirming Corollary 1.9 in this explicit model.

Example 1.28 (GOE index calculation)**.** Let M be a 1000×1000 GOE matrix and consider the shifted matrix $H = M - \mu I$. Using the semicircle law:

$$p_-(\mu) = \int_{-\infty}^{0} \frac{1}{2\pi}\sqrt{4-(\lambda+\mu)^2}\,d\lambda = \frac{1}{2} - \frac{\mu\sqrt{4-\mu^2}}{4\pi} - \frac{1}{2\pi}\arcsin\left(\frac{\mu}{2}\right) \quad \text{for } |\mu| \le 2.$$

For $\mu = 0$ (zero shift): $p_-(0) = 1/2$ — half the eigenvalues are negative (index ≈ 500).
For $\mu = 1$: $p_-(1) \approx 0.20$ — index ≈ 200.
For $\mu = 2$: $p_-(2) = 0$ — all eigenvalues positive (local minimum).

A critical point of an isotropic Gaussian field with value u corresponds to shift $\mu = u - u_0$ where $u_0 \approx -2$ (the ground state energy in $d = 1000$). Thus: critical points at $u = -2$ have $\mu \approx 0$ (index ≈ 500, bad saddle); critical points at $u = -1$ have $\mu \approx 1$ (index ≈ 200); critical points at $u = 0$ have $\mu \approx 2$ (index ≈ 0, minimum).

1.9 Open Problems

Open Problem 1: Tighter index bounds for real networks

Theorem 1.8 applies to isotropic Gaussian fields. Real network losses have strong anisotropy: the Hessian is low-rank plus bulk (Proposition 1.16). Whether the loss–index monotonicity of Corollary 1.9 holds for anisotropic fields is open. Partial results (Fyodorov and Khoruzhenko 2016) suggest it does, but a complete proof requires understanding the spectral distribution of the Hessian at critical points of non-isotropic fields.

Open Problem 2: Polynomial-time escape in practice

Theorem 1.20 guarantees polynomial-time escape in terms of gradient evaluations, but the polynomial degree depends on γ (minimum negative eigenvalue) and ρ (Hessian Lipschitz constant), both unknown and architecture-dependent. Empirical measurements of these constants across Transformer scales would give quantitative predictions for when training "gets stuck."

Open Problem 3: Saddle points in fine-tuning

During fine-tuning of pretrained LLMs, the initialisation is already near a minimum of the pretraining loss. Whether the saddle point structure of the fine-tuning loss (which is a perturbation of the pretraining loss) is well-behaved is unknown. The presence of loss of plasticity (Chapter 4) suggests that fine-tuning saddles may be qualitatively different from scratch-training saddles.

1.10 Chapter Summary

- The Morse inequalities (Theorem 1.2) give a lower bound on the number of critical points by type but not an upper bound — saddle points can be exponential.

- In high dimension, the Åufinger–Ben Arous–Černý theorem (Theorem 1.8) shows that critical points below a loss threshold are almost all local minima: high-index saddle points are exponentially suppressed at low energy.
- The strict saddle property is proved for two-layer linear networks (Theorem 1.13) and deep linear networks (Theorem 1.15); extension to non-linear networks remains open.
- Perturbed gradient descent (Theorem 1.20, proved in full) finds an ε-second-order stationary point in $O(\varepsilon^{-2}\log^4 d)$ gradient steps — dimension-free in the leading term.
- SGD with small batch size provides sufficient noise to escape strict saddles without explicit perturbation (Proposition 1.21).
- The bulk–outlier decomposition of the Hessian spectrum (Proposition 1.16) connects the theoretical index analysis to the empirical spectral structure measured in real networks.

Exercises

Exercise 1.1. Verify the Morse inequality $\sum_k (-1)^k c_k = \chi(T^2) = 0$ for the torus $T^2 = S^1 \times S^1$ using the height function $f(x, y) = \cos(2\pi x) + 2\cos(2\pi y)$. List all critical points and their indices.

Exercise 1.2. Let M be a $d \times d$ GOE matrix with $d = 100$. (a) Compute the expected number of negative eigenvalues. (b) For the shifted matrix $H = M - \mu I$ with $\mu = 1$, compute the expected index using the semicircle law formula of Example 1.28. (c) At what value of μ does the index equal $d/4$?

Exercise 1.3 (Complete proof of Kawaguchi for $L = 3$)**.** Extend Theorem 1.13 to a three-layer linear network $f = W_3 W_2 W_1 X$ with $W_i \in \mathbb{R}^{d_i \times d_{i-1}}$, $d_1 = d_2 = d_0 = d_3$. Characterise all critical points and show that non-global-minimum saddle points are strict. *(Hint: use the Du–Lee argument and the SVD of the product matrix $W_3 W_2 W_1$.)*

Exercise 1.4. In Algorithm 1, set $d = 500$, $\ell = 10$, $\rho = 1$, $\gamma = 0.1$, $\delta = 0.05$. Compute the perturbation radius r, gradient threshold g, and the upper bound on the number of gradient evaluations T to reach an $\varepsilon = 0.01$ second-order stationary point.

Exercise 1.5. Prove Proposition 1.21: show that at a strict saddle point of a generic loss function (with positive definite gradient covariance), the mini-batch SGD noise satisfies the escape condition of Theorem 1.20. What is the batch size B above which the noise is *insufficient* for escape?

Further Reading

The Morse inequalities are classical; the definitive reference is Milnor (1963), *Morse Theory*. For the Witten (1982) supersymmetric proof (which connects to the Morse complex via a Laplacian), see Jost (2008), *Riemannian Geometry and Geometric Analysis*, Chapter 8.

The Åufinger–Ben Arous–Černý theorem appears in *Annals of Probability* 41(4), 2013; an accessible introduction is the survey by Ben Arous (2021), "Random matrices and complexity of spin glasses." The GOE and Wigner semicircle law are treated in depth in Anderson, Guionnet, and Zeitouni (2010), *An Introduction to Random Matrices*.

The connection to neural network loss landscapes was popularised by Dauphin et al. (2014, NeurIPS) and formalised by Choromanska et al. (2015, AISTATS). The perturbed gradient descent result (Theorem 1.20) is from Jin, Ge, Netrapalli, Kakade, and Jordan (ICML 2017);

the sharper version with $\tilde{O}(\varepsilon^{-2})$ gradient complexity is in Jin et al. (*Mathematical Programming* 2021).

The strict saddle property for two-layer networks is proved in Kawaguchi (2016, NeurIPS). The deep linear network result is from Du and Lee (2018, ICML). A unified treatment of both appears in Bhojanapalli, Neyshabur, and Srebro (2016). The μP parametrisation is introduced in Yang and Hu (2022, NeurIPS).

1.11 Extended Numerical Analysis: The Landscape of a Two-Layer Network

This section develops a complete numerical analysis of the loss landscape of a two-layer linear network, connecting the abstract theory of Sections 1.2–1.6 to explicit computable quantities.

1.11.1 Setup

Consider the two-layer linear network:

$$f(x; W_1, W_2) = W_2 W_1 x, \quad W_1 \in \mathbb{R}^{k \times d_0}, \quad W_2 \in \mathbb{R}^{d_2 \times k},$$

with squared loss:

$$L(W_1, W_2) = \frac{1}{2n} \|W_2 W_1 X - Y\|_F^2,$$

where $X \in \mathbb{R}^{d_0 \times n}$, $Y \in \mathbb{R}^{d_2 \times n}$. We use the concrete instance $d_0 = d_2 = k = 2$, $n = 4$, with:

$$X = \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{pmatrix}, \quad Y = \begin{pmatrix} 2 & 1 & 2 & 1 \\ 1 & 3 & 1 & 3 \end{pmatrix}.$$

The least-squares solution is $W^* = YX^\dagger = YX^\top (XX^\top)^{-1}$.

Computing $XX^\top$: $XX^\top = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \cdot 2 = 2I$ (since each column of X is a standard basis vector, appearing twice).

Computing $YX^\top$: $YX^\top = \begin{pmatrix} 2 & 1 & 2 & 1 \\ 1 & 3 & 1 & 3 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 4 & 2 \\ 2 & 6 \end{pmatrix}$.

The global minimum: $W^* = YX^\top (XX^\top)^{-1} = \begin{pmatrix} 4 & 2 \\ 2 & 6 \end{pmatrix} \cdot \frac{1}{2} I = \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix}$.

Any factorisation $W_2 W_1 = W^*$ achieves $L = 0$.

1.11.2 Critical Points

By Theorem 1.13, the critical points are:

1. **Global minima** (index 0): all (W_1, W_2) with $W_2 W_1 = W^*$. The set of solutions is a manifold of dimension $k^2 = 4$ (parametrised by the invertible matrix $T \in \mathrm{GL}_k(\mathbb{R})$ via $W_1 = T^{-1}\tilde{W}_1$, $W_2 = \tilde{W}_2 T$).

2. **Strict saddle** (index > 0): the origin $W_1 = W_2 = 0$, with $L(0, 0) = \frac{1}{2n} \|Y\|_F^2$. Let us compute $\|Y\|_F^2 = 4 + 1 + 4 + 1 + 1 + 9 + 1 + 9 = 30$, so $L(0, 0) = 30/8 = 3.75$.

1.11.3 Hessian at the Saddle

At $(W_1, W_2) = (0, 0)$, the Hessian of L with respect to all parameters (W_1, W_2) can be computed by expanding the loss to second order. The parameters are $\theta = (\mathrm{vec}(W_1)^\top, \mathrm{vec}(W_2)^\top)^\top \in \mathbb{R}^{d_0 k + k d_2} = \mathbb{R}^{4+4} = \mathbb{R}^8$.

The second-order Taylor expansion of $L(\theta)$ around $\theta = 0$:

$$L(\theta) \approx L(0) + \theta^\top H \theta / 2,$$

where $H_{ij} = \left. \frac{\partial^2 L}{\partial \theta_i \partial \theta_j} \right|_{\theta = 0}$.

Direct computation gives:

$$\frac{\partial^2 L}{\partial W_{2,ab}\partial W_{1,cd}}\bigg|_{W=0} = \frac{1}{n}[XX^\top]_{dc}\cdot\delta_{ab} \quad \text{(using } W_2=0,\, W_1=0\text{)},$$

... wait, at $W_1 = W_2 = 0$: $\frac{\partial L}{\partial W_2} = \frac{1}{n}RX^\top W_1^\top = 0$ (since $W_1 = 0$), and $\frac{\partial^2 L}{\partial W_2^2}|_0 = 0$ (quadratic in W_1, which is 0). The non-trivial second derivatives are $\frac{\partial^2 L}{\partial W_2 \partial W_1}$:

$$\frac{\partial^2 L}{\partial (W_2)_{ab}\,\partial (W_1)_{cd}}\bigg|_0 = -\frac{1}{n}(YX^\top)_{ad}\,\delta_{bc} + \frac{1}{n}\delta_{ac}(XX^\top)_{dc}\cdot 0 = 0\cdot\ldots$$

Let us be more careful. $L = \frac{1}{2n}\|W_2W_1X - Y\|_F^2$. Denote $P = W_2W_1X \in \mathbb{R}^{d_2\times n}$. Then $L = \frac{1}{2n}\|P - Y\|_F^2$.

$$\frac{\partial L}{\partial W_1} = \frac{1}{n}W_2^\top(W_2W_1X - Y)X^\top.$$

At $W_1 = W_2 = 0$: $\frac{\partial L}{\partial W_1}\big|_0 = \frac{1}{n}\cdot 0\cdot(-Y)X^\top = 0$. ✓

Second derivative with respect to W_1 entries:

$$\frac{\partial^2 L}{\partial (W_1)_{ab}\,\partial (W_1)_{cd}}\bigg|_0 = \frac{1}{n}(W_2^\top W_2)_{ca}\,(XX^\top)_{db}\bigg|_{W_2=0} = 0.$$

Second derivative with respect to W_2 entries:

$$\frac{\partial^2 L}{\partial (W_2)_{ab}\,\partial (W_2)_{cd}}\bigg|_0 = \frac{1}{n}(W_1XX^\top W_1^\top)_{ca}\,\delta_{bd}\bigg|_{W_1=0} = 0.$$

Mixed:

$$\frac{\partial^2 L}{\partial (W_2)_{ab}\,\partial (W_1)_{cd}}\bigg|_0 = \frac{1}{n}\frac{\partial}{\partial (W_2)_{ab}}[W_2^\top(W_2W_1X - Y)X^\top]_{cd}\bigg|_0.$$

Expanding: $[W_2^\top(W_2W_1X - Y)X^\top]_{cd} = \sum_e (W_2)_{ec}[(W_2W_1)_{ef}X_{fd} - Y_{ef}]X_{gd}\cdots$

Simpler: at $W_1 = W_2 = 0$, the Hessian has blocks:

$$H = \begin{pmatrix} H_{11} & H_{12} \\ H_{12}^\top & H_{22}\end{pmatrix} = \begin{pmatrix} 0 & H_{12} \\ H_{12}^\top & 0\end{pmatrix},$$

where H_{12} encodes the mixed second derivatives. The eigenvalues of H come in $\pm$ pairs from the off-diagonal block structure, giving indices 0, ..., $d/2$ negative eigenvalues. In our 8×8 case, the mixed block H_{12} has rank 4 (for generic data), giving 4 positive and 4 negative eigenvalues — index = 4 at the origin saddle.

Index verification against Theorem 1.13: The origin is a strict saddle (index > 0), consistent with Theorem 1.13 since $W_1 = W_2 = 0$ gives $L > 0$.

1.11.4 Escape from the Saddle: Explicit Trajectory

The escape direction is the eigenvector v_- corresponding to the most negative eigenvalue of H at the origin. For the block structure $H = \begin{pmatrix} 0 & C \\ C^\top & 0\end{pmatrix}$, the eigenvectors of H are $\begin{pmatrix} u \\ \pm v\end{pmatrix}$ where (u, v) are left and right singular vectors of C, with eigenvalues $\pm\sigma_i(C)$.

The most negative eigenvalue is $-\sigma_{\max}(C)$, with eigenvector $\begin{pmatrix} u_1 \\ -v_1\end{pmatrix}$ where u_1, v_1 are the leading left/right singular vectors of $C = H_{12}$.

Gradient descent from $\theta_0 = \varepsilon(u_1^\top, -v_1^\top)^\top$ (a small perturbation in the direction of v_-) will escape the saddle at rate $\Omega(\varepsilon^2\sigma_{\max}(C)t)$, reaching a global minimum in time $O(1/(\varepsilon\sigma_{\max}(C)))$.

This is the explicit version of the argument in Proposition 1.18 and Theorem 1.20: the escape direction is the most negative Hessian eigenvector, and the escape rate is controlled by the magnitude of the negative eigenvalue.

1.11.5 Condition Number and Adam's Advantage

At the global minimum $W^* = \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix}$, the Hessian can be computed as:

$$H|_{W^*} = \frac{1}{n} \begin{pmatrix} (W_2^*)^\top W_2^* \otimes XX^\top & 0 \\ 0 & W_1^* XX^\top (W_1^*)^\top \otimes I \end{pmatrix},$$

(using the Kronecker product formula for the Hessian of matrix factorisation losses). With $XX^\top = 2I$ and any factorisation $W_1^* W_2^* = W^*$, the Hessian blocks have eigenvalues proportional to $\sigma_i(W^*)^2 \cdot 2/n$.

The singular values of $W^* = \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix}$: $\sigma_1 = \frac{3+\sqrt{5}}{2} \approx 2.62$, $\sigma_2 = \frac{3-\sqrt{5}}{2} \approx 0.38$.

Condition number: $\kappa = (\sigma_1/\sigma_2)^2 \approx (2.62/0.38)^2 \approx 47.5$.

For SGD, the optimal learning rate is $\eta^* = 1/\lambda_{\max}(H) \propto 1/\sigma_1^2$, and the convergence rate is $(1 - \eta^* \lambda_{\min}^+)^t \approx (1 - 1/\kappa)^t \approx e^{-t/47.5}$. After 100 steps, SGD has made progress $1 - e^{-100/47.5} \approx 88\%$ of the way.

For Adam with $\hat{v}_{t,i} \approx \sigma_i^2 \cdot 2/n$: the effective learning rate in direction i is $\eta/\hat{v}_{t,i}^{1/2} \propto \eta n/(2\sigma_i)$, which is the *same* for all directions (since Adam normalises by the gradient scale). Adam's effective condition number is thus approximately 1 — full-step convergence in all directions. After 100 steps, Adam has made $\approx 100\%$ progress regardless of κ.

1.11.6 Summary of the Explicit Example

Property	Value
Global minimum loss L^*	0
Saddle point loss $L(0,0)$	3.75
Index of saddle at origin	4 (of 8 Hessian eigenvectors)
Singular values of W^*	≈ 2.62, 0.38
Condition number κ	≈ 47.5
SGD convergence rate	$e^{-t/47.5}$
Adam convergence rate	approximately e^{-t} (condition-number-free)

Table 1.2: Summary of the two-layer network example.

1.12 Deep Dive: The Topology of Loss Basins

This section develops the topological theory of loss basins more completely, connecting the Morse-theoretic counting of critical points to the practical behaviour of gradient descent trajectories.

1.12.1 The Stable and Unstable Manifolds

At a hyperbolic critical point w^* (all Hessian eigenvalues non-zero), the stable and unstable manifolds partition the neighbourhood into four quadrants.

Definition 1.29 (Stable and unstable manifolds)**.** Let w^* be a hyperbolic critical point of L. The *stable manifold* $W^s(w^*)$ and *unstable manifold* $W^u(w^*)$ of the gradient flow $\dot{w} = -\nabla L(w)$ are:

$$W^s(w^*) = \{w : \lim_{t \to +\infty} \phi_t(w) = w^*\},$$
$$W^u(w^*) = \{w : \lim_{t \to -\infty} \phi_t(w) = w^*\},$$

where ϕ_t is the gradient flow. The stable manifold has dimension $d - \text{index}(w^*)$ (the number of positive Hessian eigenvalues), and the unstable manifold has dimension $\text{index}(w^*)$.

Proposition 1.30 (Stable manifold theorem for gradient flows)**.** *Near a hyperbolic critical point w^* of L, the stable and unstable manifolds are C^k submanifolds of $\mathbb{R}^d$ (for $L \in C^{k+1}$), tangent to the positive and negative eigenspaces of $\nabla^2 L(w^*)$ respectively. They intersect transversally at w^*.*

Proof. This is the Stable Manifold Theorem for autonomous ODEs, applied to the gradient flow $\dot{w} = -\nabla L(w)$. The linearisation at w^* is the linear system $\dot{\delta w} = -\nabla^2 L(w^*)\delta w$. By hyperbolicity, this has no purely imaginary eigenvalues (equivalently: $\nabla^2 L(w^*)$ has no zero eigenvalues). The Stable Manifold Theorem (Hartman–Grobman) then guarantees the existence of C^k stable and unstable manifolds tangent to the positive and negative eigenspaces. For C^{k+1} vector fields (i.e., C^{k+1} loss functions), the manifolds are C^k. □

Remark 1.31. The stable manifold at a strict saddle has measure zero (dimension $< d$), so a random initialisation will not land on it with probability 1. However, near-symmetric initialisations (constant initialisation, or weight-sharing in symmetric architectures) can place iterates near the stable manifold, causing slow escape. The Morse lemma (used in the proof of Theorem 1.2) shows that near w^*, the loss is equivalent (up to smooth change of variables) to the standard quadratic $-\sum_{i=1}^{k} u_i^2 + \sum_{i=k+1}^{d} u_i^2$, so the stable manifold is locally the coordinate subspace $\{u_1 = \cdots = u_k = 0\}$. Symmetric initialisations that place w_0 in this subspace are exactly those where the symmetry of the network forces $u_1(0) = \cdots = u_k(0) = 0$.

1.12.2 The Morse Complex and the Betti Numbers

The Morse complex provides a cell decomposition of the parameter space, with cells corresponding to critical points and boundaries given by gradient flow lines between them.

Definition 1.32 (Morse complex)**.** The *Morse complex* $\text{CM}_*(L)$ is the chain complex with:

- CM_k = free abelian group generated by index-k critical points of L.
- Boundary map $\partial_k : \text{CM}_k \to \text{CM}_{k-1}$ defined by: $\partial_k(w^*) = \sum_{v^*:\, \text{index}(v^*)=k-1} n(w^*, v^*) \cdot v^*$, where $n(w^*, v^*)$ counts gradient flow lines from w^* to v^* with sign (determined by the orientation of the unstable manifold).

Theorem 1.33 (Morse homology)**.** $H_k(\text{CM}_*(L)) \cong H_k(M; \mathbb{Z})$ *(singular homology with integer coefficients).*

This is the fundamental theorem connecting the Morse complex to topology. For the specific application to neural networks on $M = \mathbb{R}^d$ (or a compact manifold after layer normalisation), it gives:

$$\beta_0 = \dim H_0 = \text{number of connected components of } \{L \le u^*\} = 1 \text{ (connected)},$$
$$\beta_1 = \dim H_1 = 0 \text{ (simply connected for } \mathbb{R}^d).$$

The weak Morse inequalities $c_k \ge \beta_k$ then give:

- $c_0 \ge 1$: at least one local minimum (guaranteed).
- $c_1 \ge 0$: no lower bound on index-1 saddles.
- The alternating sum $c_0 - c_1 + c_2 - \cdots = \chi(\mathbb{R}^d) = 1$: a topological constraint.

1.12.3 Basin Geometry and the Gromov–Hausdorff Perspective

From the practical perspective of gradient descent, the relevant question is not the total number of critical points but the *basin structure*: the partition of parameter space into basins of attraction of different minima.

Definition 1.34 (Basin of attraction)**.** The *basin of attraction* of a local minimum w_j^* under gradient flow is:

$$\mathcal{B}(w_j^*) = \{w : \lim_{t\to\infty} \phi_t(w) = w_j^*\} = W^s(w_j^*) \setminus \{w_j^*\}.$$

The basins partition $\mathbb{R}^d$ up to the stable manifolds of saddle points (which have measure zero).

Proposition 1.35 (Basin size and sharpness)**.** *For a local minimum w^* with Hessian $H = \nabla^2 L(w^*)$, the* volume *of the basin $\mathcal{B}(w^*)$ within a ball of radius R is approximately:*

$$\mathrm{Vol}(\mathcal{B}(w^*) \cap \mathcal{B}(0, R)) \approx \frac{C_d R^d}{\sqrt{\det H}},$$

where C_d is the volume of the d-dimensional unit ball and the approximation holds when $R \gg \left\|H^{-1/2}\right\|$ (the basin is "large compared to the local curvature").

Proof. Near w^*, the level set $\{L(w) = L(w^*) + \varepsilon\}$ is an ellipsoid with principal radii $\sqrt{2\varepsilon/\lambda_i}$ (from the quadratic approximation). The volume enclosed is $\prod_i \sqrt{2\varepsilon/\lambda_i} \cdot \omega_d = (2\varepsilon)^{d/2}\omega_d/\sqrt{\det H}$. Integrating over ε from 0 to the saddle height gives the basin volume proportional to $1/\sqrt{\det H}$. □

Remark 1.36. Proposition 1.35 has an important implication: the basin volume is inversely proportional to $\sqrt{\det H} = \prod_i \lambda_i$ (the product of eigenvalues). A flat minimum (small λ_i) has a *larger* basin, meaning:

- Random initialisation is more likely to fall into the flat minimum's basin.
- Small perturbations of the initialisation are more likely to stay in the basin.
- SGD with noise (small batch) is more likely to find the flat minimum, because the noise has a larger target to hit.

This is the topological basis for the empirical observation that SGD with small batch size finds flatter minima: the noise steers the iterate toward the larger basins, which are exactly the flatter minima. SAM makes this implicit bias explicit.

1.12.4 The Lojasiewicz Inequality and Global Convergence

The Łojasiewicz inequality is a powerful tool for proving that gradient descent converges to a critical point (not just that gradient norms go to zero).

Theorem 1.37 (Łojasiewicz inequality)**.** *Let $L : \mathbb{R}^d \to \mathbb{R}$ be a real analytic function and let w^* be a critical point. Then there exist $\varepsilon, C, \theta \in (0, 1/2]$ such that for all w with $\|w - w^*\| < \varepsilon$:*

$$|L(w) - L(w^*)|^\theta \le C \left\|\nabla L(w)\right\|.$$

Corollary 1.38 (Global convergence of gradient descent for analytic losses)**.** *Let L be a real analytic function (e.g., a polynomial network with polynomial activation). Then the gradient descent trajectory w_t converges to a critical point w^* as $t \to \infty$ (provided the iterates are bounded).*

Proof. The Łojasiewicz inequality with exponent θ gives: $\|\nabla L(w_t)\| \geq C^{-1}|L(w_t) - L(w^*)|^\theta$. The gradient descent update gives $L(w_{t+1}) \leq L(w_t) - \frac{\eta}{2}\|\nabla L(w_t)\|^2$. Combining: $L(w_t) - L(w_{t+1}) \geq \frac{\eta C^{-2}}{2}|L(w_t) - L(w^*)|^{2\theta}$.

For $\theta \leq 1/2$ (the typical case), $2\theta \leq 1$, and the loss gap $L(w_t) - L(w^*)$ decreases at a rate that guarantees $\sum_t \|w_t - w_{t+1}\| < \infty$, hence $\{w_t\}$ is Cauchy and converges to a limit w^*. Since the limit satisfies $\nabla L(w^*) = 0$, it is a critical point. □

Remark 1.39. The Łojasiewicz inequality is why gradient descent converges for polynomial (or analytic) network losses, even though such losses may have an exponential number of saddle points. The key: once the iterate is near a critical point, the loss decreases at a rate controlled by the Łojasiewicz exponent θ. For $\theta = 1/2$ (the generic case for Morse functions), the convergence is exponential; for $\theta < 1/2$, it is polynomial.

1.12.5 Connecting Saddle Points to Generalisation: The Loss Plateau

An important empirical observation (Goodfellow et al., 2015; Fort and Scherlis, 2019) is that the loss landscape of deep networks has a characteristic "plateau" structure at high loss values: the loss surface is locally flat in many directions, with a few steeply descending directions. This plateau corresponds, in the language of Chapter 1, to a region of high-index saddle points.

Proposition 1.40 (Gradient norm in the plateau region)**.** *Let L be a smooth loss satisfying the Łojasiewicz inequality with exponent $\theta < 1/2$. In the plateau region $\{w : L(w) \geq L^* + \Delta\}$ (far from the minimum), the gradient norm satisfies:*

$$\|\nabla L(w)\| \leq C|L(w) - L^*|^\theta \leq C(L(w) - L^*)^\theta,$$

giving a slow decrease rate. Specifically, in the plateau, the gradient is bounded by $C\Delta^\theta$ even though the loss is Δ above the minimum — the loss is "high but gradient is small", which is the signature of a flat plateau.

This explains the slow initial phase of training: the loss is high (plateau), the gradient is small (flat region), and gradient descent makes slow progress. The loss decreases abruptly once the iterate descends from the plateau into a basin (the "grokking" phenomenon in some settings). The analysis of Theorem 1.20 (PGD escapes in polynomial time) applies precisely to this phase: the strict saddle property ensures that the plateau can be escaped in polynomial time via the noise of SGD.

1.13 The Random Field Model: Detailed Calculations

This section works through the Kac–Rice computation of Theorem 1.8 in sufficient detail to make it reproducible.

1.13.1 Setup of the Kac–Rice Formula

Let $f : \mathbb{R}^d \to \mathbb{R}$ be an isotropic Gaussian random field with covariance $K(r) = \mathbb{E}[f(x)f(y)]$ where $r = \|x - y\|$. Write $\mu = K(0) = \mathbb{E}[f^2]$ (variance) and $\kappa_1 = -K''(0)/d$ (related to the gradient variance: $\mathbb{E}[|\partial_i f|^2] = -K''(0) = d\kappa_1$).

The Kac–Rice formula for the expected number of critical points with value $\leq u$ is:

$$\mathbb{E}[C(u)] = \int_{\mathbb{R}^d} \mathbb{E}\big[|\det \nabla^2 f(x)| \cdot \mathbf{1}_{f(x)\leq u}\big] \cdot p_{\nabla f(x)}(0)\, d^d x,$$

where $p_{\nabla f(x)}(0)$ is the density of $\nabla f(x)$ evaluated at 0.

1.13.2 Simplification via Isotropy

For an isotropic field, all x are equivalent (by stationarity and isotropy), so:

$$\mathbb{E}[C(u)] = \mathrm{Vol}(M) \cdot \mathbb{E}\big[|\det \nabla^2 f(x)| \cdot \mathbf{1}_{f(x)\le u}\big]_{x=0} \cdot p_{\nabla f(0)}(0).$$

The gradient $\nabla f(0)$ is a d-dimensional Gaussian with covariance $d\kappa_1 I$. Its density at 0 is:

$$p_{\nabla f(0)}(0) = (2\pi d\kappa_1)^{-d/2}.$$

1.13.3 Distribution of the Hessian at a Critical Point

Conditioning on $f(0) = u$ and $\nabla f(0) = 0$, the Hessian $\nabla^2 f(0)$ has distribution:

$$\nabla^2 f(0) \,|\, f(0) = u, \nabla f(0) = 0 \overset{d}{=} c_1 M + c_2 u I,$$

where M is a GOE matrix and c_1, c_2 are constants depending on the covariance function:

$$c_1 = \sqrt{K''''(0)/d - K''(0)^2/(\mu d)}, \qquad c_2 = K''(0)/(\mu d).$$

(This follows from the general theory of conditional distributions for Gaussian processes: the mean of the Hessian given the value at a point is a multiple of the identity, and the residual is isotropic.)

1.13.4 Computing the Expected Determinant

By the Wigner semicircle law (Theorem 1.6):

$$\frac{1}{d}\log|\det(c_1 M + c_2 u I)| \to \int_{-2}^{2} \log|c_1\lambda + c_2 u| \rho_{\mathrm{sc}}(\lambda)\, d\lambda.$$

This integral can be computed explicitly using the Stieltjes transform of the semicircle:

$$\int \log|c_1\lambda + c_2 u|\, \rho_{\mathrm{sc}}(\lambda)\, d\lambda = \begin{cases} \log(c_2|u|/2) & \text{if } c_2|u| > 2c_1 \text{ (all eigenvalues same sign)} \\ \log(c_1) + \frac{1}{2}\log\left(\frac{c_2^2 u^2}{4c_1^2} - 1\right) + \text{const} & \text{otherwise (mixed signs)} \end{cases}$$

The complexity function $\Theta_k(u)$ in Theorem 1.8 is:

$$\Theta_k(u) = -\frac{d}{2}\log(2\pi d\kappa_1) + \int \log|c_1\lambda + c_2 u|\, \rho_{\mathrm{sc}}(\lambda)\, d\lambda + \frac{1}{2}\log(d/2\pi) - k\cdot\log(2) + \text{const},$$

where the last term $-k\log 2$ comes from the probability that a random GOE matrix has exactly k negative eigenvalues (which is 2^{-d} times a binomial factor).

The key inequality $\Theta_k(u) < \Theta_0(u)$ for $k \ge \delta d$ follows from the strict increase of $\int \log|c_1\lambda + c_2 u|\, \rho_{\mathrm{sc}}$ as a function of u (controlling the expected determinant magnitude) combined with the $-k\log 2$ penalty for having many negative eigenvalues.

Example 1.41 (Explicit complexity for the spherical p-spin model)**.** For the pure p-spin spherical model $f(x) = \sum_{i_1,\dots,i_p} J_{i_1\dots i_p} x_{i_1}\cdots x_{i_p}$ (a canonical model in statistical physics), the covariance is $K(r) = r^p$. With $K(0) = 1$, $K''(0) = p(p-1)$, the constants are $c_1 = \sqrt{p(p-1)/d}$ and $c_2 = (p-1)/\sqrt{d}$. For $p = 2$ (quadratic spin glass): $c_1 = \sqrt{2/d}$, $c_2 = 1/\sqrt{d}$, and the complexity function gives $\Theta_0(u) = -u^2/2 + \text{const}$ for $|u| < 2$ — matching the known result that the ground state energy is $u_0 = -2$ and all critical points with $u > -2$ are saddles.

Chapter 2

Adam, AdamW, and the Theory of Adaptive Optimisers

Adam is not just a faster gradient descent. It is a different algorithm with a different implicit bias — one that sometimes agrees with SGD, sometimes contradicts it, and is never quite the same thing.

2.1 The Failure of Vanilla Gradient Descent

Gradient descent with a fixed learning rate η updates parameters as:

$$w_{t+1} = w_t - \eta g_t, \qquad g_t = \nabla L(w_t).$$

Its convergence rate for an ℓ-smooth non-convex function is $O(\ell\Delta_f/T)$ per gradient step. The learning rate must satisfy $\eta \leq 1/\ell$.

Definition 2.1 (Condition number of the loss)**.** The condition number of L at w is:

$$\kappa(w) = \frac{\lambda_{\max}(\nabla^2 L(w))}{\lambda^+_{\min}(\nabla^2 L(w))},$$

where $\lambda^+_{\min}$ denotes the smallest strictly positive eigenvalue. Gradient descent achieves convergence rate $O(\kappa)$ in the strongly convex case.

Example 2.2 (Condition number in a two-layer linear network)**.** Consider the loss $L(w_1, w_2) = \frac{1}{2}(w_2 w_1 - y)^2$ for scalars w_1, w_2, y. The Hessian at (w_1, w_2) is:

$$H = \begin{pmatrix} w_2^2 & 2w_1 w_2 - y \\ 2w_1 w_2 - y & w_1^2 \end{pmatrix}.$$

At the saddle $(0,0)$: $H = 0$ (degenerate). At the minimum $(1, y)$ (if $y > 0$): $H = \begin{pmatrix} y^2 & y \\ y & 1 \end{pmatrix}$, with eigenvalues $\frac{1+y^2 \pm \sqrt{(1+y^2)^2-4}}{2}$. For large y: $\lambda_{\max} \approx y^2$, $\lambda_{\min} \approx 1/y^2$, giving $\kappa \approx y^4$. For $y = 10$, this is $\kappa \approx 10^4$, requiring $\eta \leq 10^{-2}$ — tiny for a scalar problem. This is the ill-conditioning that adaptive methods resolve.

Geometric Intuition

In a network with embedding weights (updated by rare, sparse gradients) and feedforward weights (updated by dense gradients), the condition number κ is the ratio of the largest to smallest "typical gradient magnitudes squared." If embeddings receive gradients of magnitude 10^{-3} and feedforward weights receive 10^{-1}, then $\kappa \approx 10^4$, and a global learning rate must be $\eta \leq 10^{-1}/\ell$ — too small for embeddings to learn fast. Adaptive optimisers resolve this by giving each parameter its own effective learning rate.

2.2 From Online Mirror Descent to Adam

2.2.1 Online Mirror Descent and Adaptive Regularisation

Definition 2.3 (Online Mirror Descent)**.** Given a sequence of loss functions $f_1, f_2, \ldots$, *Online Mirror Descent* (OMD) with Bregman divergence D_ψ generated by a strongly convex ψ solves at each step:

$$w_{t+1} = \arg\min_w \left[\langle g_t,\, w\rangle + \frac{1}{\eta} D_\psi(w, w_t) \right], \quad g_t = \nabla f_t(w_t).$$

For $\psi(w) = \frac{1}{2}\|w\|_2^2$: $D_\psi(w, w') = \frac{1}{2}\|w - w'\|^2$ and OMD reduces to gradient descent.

AdaGrad (Duchi, Hazan, and Singer, 2011) corresponds to OMD with the adaptive Bregman divergence generated by $\psi_t(w) = \frac{1}{2}\|w\|_{H_t}^2$, where:

$$H_t = \operatorname{diag}\left(\sqrt{\sum_{s=1}^{t} g_{s,i}^2} \right)_{i=1}^{d}.$$

The AdaGrad update is:

$$w_{t+1,i} = w_{t,i} - \frac{\eta}{\sqrt{\sum_{s=1}^{t} g_{s,i}^2}}\, g_{t,i}.$$

Proposition 2.4 (AdaGrad regret bound)**.** *For any sequence of convex loss functions $f_1, \ldots, f_T$ and any $w^* \in \mathbb{R}^d$:*

$$\sum_{t=1}^{T} f_t(w_t) - \sum_{t=1}^{T} f_t(w^*) \leq \frac{\|w_1 - w^*\|^2}{2\eta} \sum_{i=1}^{d} \sqrt{\sum_{t=1}^{T} g_{t,i}^2}.$$

For sparse gradients (many $g_{t,i} = 0$), the right-hand side is much smaller than the $O(d\sqrt{T})$ bound of gradient descent — AdaGrad is "dimension-free" for sparse problems.

Proof. By the definition of OMD with the adaptive Bregman divergence, the one-step regret satisfies:

$$f_t(w_t) - f_t(w^*) \leq \langle g_t,\, w_t - w^*\rangle = \langle H_t(w_t - w_{t+1}),\, w_t - w^*\rangle + \langle g_t - H_t(w_t - w_{t+1}),\, w_t - w^*\rangle\,.$$

The first term telescopes via the three-point identity for Bregman divergences:

$$\sum_{t=1}^{T} \langle H_t(w_t - w_{t+1}),\, w_t - w^*\rangle \leq \frac{1}{2\eta}\|w_1 - w^*\|_{H_T}^2 + \frac{\eta}{2}\sum_{t=1}^{T} \|g_t\|_{H_t^{-1}}^2\,.$$

Since $H_t = \operatorname{diag}(\sqrt{\sum_{s=1}^{t} g_{s,i}^2})$, we have $\|g_t\|_{H_t^{-1}}^2 = \sum_i g_{t,i}^2 / \sqrt{\sum_{s=1}^{t} g_{s,i}^2} \leq 2(\sqrt{\sum_{s=1}^{t} g_{s,i}^2} - \sqrt{\sum_{s=1}^{t-1} g_{s,i}^2})$. Summing over t, this telescopes to $2\sum_i \sqrt{\sum_{t=1}^{T} g_{t,i}^2}$. Combining gives the stated bound. □

2.2.2 The Adam Algorithm: Exponential Moving Averages

Adam (Kingma and Ba, 2015) replaces the cumulative sum in AdaGrad with an exponentially weighted moving average, addressing the problem that $\sum_{s=1}^{t} g_{s,i}^2 \to \infty$ for stationary problems (driving the learning rate to zero).

Definition 2.5 (Adam update)**.** Given learning rate η, coefficients $\beta_1, \beta_2 \in [0, 1)$, and stabiliser $\varepsilon > 0$, the Adam update at step t is:

$$\begin{aligned} m_t &= \beta_1 m_{t-1} + (1-\beta_1) g_t && \text{(first moment)} \\ v_t &= \beta_2 v_{t-1} + (1-\beta_2) g_t^2 && \text{(second moment)} \\ \hat{m}_t &= m_t / (1-\beta_1^t) && \text{(bias correction)} \\ \hat{v}_t &= v_t / (1-\beta_2^t) && \text{(bias correction)} \\ w_{t+1} &= w_t - \eta\, \hat{m}_t / (\sqrt{\hat{v}_t} + \varepsilon) && \text{(update)} \end{aligned}$$

where all operations on vectors are element-wise, $g_t^2 := g_t \odot g_t$, and typical values are $\beta_1 = 0.9$, $\beta_2 = 0.999$, $\varepsilon = 10^{-8}$.

Example 2.6 (Bias correction is essential at the start)**.** Suppose $g_t = g$ is constant for all t. Without bias correction: $m_t = (1-\beta_1^t)g$, so $m_1 = 0.1g$ (10% of the true gradient at step 1). With bias correction: $\hat{m}_t = (1-\beta_1^t)g/(1-\beta_1^t) = g$ (exact). Similarly for v_t with $\beta_2 = 0.999$: at step $t = 1$, $v_1 = 0.001 g^2$, so $\sqrt{v_1} \approx 0.032|g|$ (underestimate by factor 31), while $\hat{v}_1 = 0.001 g^2 / 0.001 = g^2$ (exact). The bias correction prevents the effective learning rate from being artificially inflated in early steps.

2.2.3 Adam as Diagonally Preconditioned Mirror Descent

The update step of Adam can be written as:

$$w_{t+1} = w_t - \eta P_t^{-1} g_t, \qquad P_t = \operatorname{diag}\Big(\sqrt{\hat{v}_t} + \varepsilon\Big),$$

treating the first moment as an approximate gradient. This is gradient descent with a diagonal preconditioner P_t^{-1}: the learning rate in direction i is scaled by $(\hat{v}_{t,i}^{1/2} + \varepsilon)^{-1}$, inversely proportional to the root-mean-square of past gradients in that direction.

Remark 2.7. When $\beta_1 \to 0$ and $\beta_2 \to 0$: Adam reduces to signed gradient descent (the sign of the gradient), because $m_t \approx g_t$ and $v_t \approx g_t^2$, so $m_t / \sqrt{v_t} = \operatorname{sgn}(g_t)$.
When $\beta_2 \to 1$: Adam approaches a diagonalised version of AdaGrad.
The typical parameter choice $\beta_2 = 0.999$ gives an exponential memory of approximately $1/(1-0.999) = 1000$ steps — Adam "remembers" the last 1000 gradient magnitudes when estimating curvature.

2.3 The AMSGrad Fix: Convergence Failure of Adam

2.3.1 Adam Is Not Guaranteed to Converge

Theorem 2.8 (Reddi–Kale–Kumar 2018: Adam can diverge)**.** *There exists a sequence of convex online loss functions and a choice of β_1, β_2 such that the Adam iterates diverge to $+\infty$.*

Construction of a counter-example. Consider the one-dimensional problem with loss sequence:

$$f_t(x) = \begin{cases} Cx & \text{if } t \equiv 0 \pmod 3 \\ -x & \text{otherwise} \end{cases}$$

with $C > 2$ and $\beta_1 = 0$. The gradients are $g_t = C$ when $t \equiv 0 \pmod 3$ and $g_t = -1$ otherwise.

After $3k$ steps, the second moment estimate is approximately:

$$v_{3k} \approx \frac{(1-\beta_2)}{1-\beta_2^{3k}} \sum_{j=0}^{3k-1} \beta_2^{3k-1-j} g_j^2.$$

Since $C > 2$, the squared gradient C^2 is much larger than 1, so v_{3k} is dominated by the C^2 terms. Specifically, if $\beta_2 = 1 - \delta$ for small $\delta > 0$:

$$v_{3k} \approx \frac{1-(1-\delta)^3}{3} \cdot C^2 + \text{smaller terms} \approx \delta C^2.$$

Meanwhile, the effective step size in the negative direction (when $g_t = -1$) is:

$$\frac{\eta |g_t|}{\sqrt{v_t} + \varepsilon} \approx \frac{\eta}{\sqrt{\delta} C}.$$

And in the positive direction (when $g_t = C$):

$$\frac{\eta C}{\sqrt{v_t} + \varepsilon} \approx \frac{\eta C}{\sqrt{\delta} C} = \frac{\eta}{\sqrt{\delta}}.$$

The net movement per 3-step cycle is:

$$\frac{\eta C}{\sqrt{\delta} C} - 2 \cdot \frac{\eta}{\sqrt{\delta} C} = \frac{\eta}{\sqrt{\delta}} \left(1 - \frac{2}{C}\right) > 0$$

since $C > 2$. So the iterate moves in the positive direction each cycle, away from the optimum $x^* = 0$. As $t \to \infty$, $w_t \to +\infty$. □

Remark 2.9. The root cause: the exponential moving average in v_t can cause the effective step size in a beneficial direction to *increase* during a sequence of bad steps. The counter-example is adversarial; on smooth, stationary objectives, Adam converges empirically. But the theoretical failure motivates the AMSGrad fix.

2.3.2 AMSGrad: A Monotone Fix

Definition 2.10 (AMSGrad)**.** AMSGrad replaces $\hat{v}_t$ in Adam with its running maximum:

$$\begin{aligned} v_t &= \beta_2 v_{t-1} + (1-\beta_2) g_t^2 \\ \hat{v}_t &= \max(\hat{v}_{t-1}, v_t) \quad \text{(coordinate-wise)} \\ w_{t+1} &= w_t - \eta m_t / (\sqrt{\hat{v}_t} + \varepsilon). \end{aligned}$$

The maximum operation ensures $\hat{v}_{t,i}$ is non-decreasing in t for each i.

Theorem 2.11 (AMSGrad convergence, Reddi et al. 2018)**.** *Let L be convex and let $\{w_t\}$ be the AMSGrad iterates with step sizes $\eta_t = \eta/\sqrt{t}$. Then the regret satisfies:*

$$\sum_{t=1}^{T} f_t(w_t) - \sum_{t=1}^{T} f_t(w^*) \le \frac{\|w_1 - w^*\|^2}{2\eta} \sum_{i=1}^{d} \hat{v}_{T,i}^{1/2} + \sum_{i=1}^{d} \sum_{t=1}^{T} \frac{\eta^2 g_{t,i}^2}{\hat{v}_{t,i}^{1/2}}.$$

Proof. The proof follows the AdaGrad analysis (Proposition 2.4) with H_t replaced by $\operatorname{diag}(\hat{v}_t^{1/2})$.

By convexity: $f_t(w_t) - f_t(w^*) \le \langle g_t, w_t - w^* \rangle$. The AMSGrad update satisfies: $w_{t+1} = w_t - \eta_t P_t^{-1} g_t$ with $P_t = \operatorname{diag}(\hat{v}_t^{1/2} + \varepsilon)$.

Using the three-point identity for the Euclidean divergence with the weighted norm $\|\cdot\|_{P_t}$:

$$\langle g_t,\, w_t - w^*\rangle = \frac{1}{\eta_t}\langle P_t(w_t - w_{t+1}),\, w_t - w^*\rangle \le \frac{1}{2\eta_t}\left(\|w_t - w^*\|_{P_t}^2 - \|w_{t+1} - w^*\|_{P_t}^2 + \|w_t - w_{t+1}\|_{P_t}^2\right).$$

Since $\hat{v}_{t,i}$ is non-decreasing, $\|w - w^*\|_{P_t}^2 \le \|w - w^*\|_{P_{t+1}}^2$ coordinate-wise, so the telescoping gives:

$$\sum_{t=1}^{T} \frac{1}{2\eta_t}\left(\|w_t - w^*\|_{P_t}^2 - \|w_{t+1} - w^*\|_{P_t}^2\right) \le \frac{1}{2\eta_1}\|w_1 - w^*\|_{P_T}^2 = \frac{1}{2\eta}\|w_1 - w^*\|_{P_T}^2\sqrt{T}.$$

The term $\sum_t \frac{1}{2\eta_t}\|w_t - w_{t+1}\|_{P_t}^2$ equals $\sum_t \frac{\eta_t}{2}\|g_t\|_{P_t^{-1}}^2 = \sum_t \frac{\eta}{2\sqrt{t}}\sum_i \frac{g_{t,i}^2}{\hat{v}_{t,i}^{1/2}}$, giving the second term in the bound. □

2.4 AdamW: Weight Decay Done Correctly

2.4.1 Non-equivalence of L2 Regularisation and Weight Decay

Proposition 2.12 (Non-equivalence for Adam)**.** *For vanilla gradient descent, L_2-regularised training (penalising $\frac{\lambda}{2}\|w\|^2$) is identical to weight decay (multiplying w by $(1-\eta\lambda)$ at each step): both give $w_{t+1} = w_t - \eta(\nabla L(w_t) + \lambda w_t) = (1-\eta\lambda)w_t - \eta\nabla L(w_t)$. For Adam, they are not equivalent. Specifically, the L_2-regularised Adam update is:*

$$w_{t+1,i} = w_{t,i} - \frac{\eta}{\hat{v}_{t,i}^{1/2} + \varepsilon}(\hat{m}_{t,i} + \lambda w_{t,i}),$$

while weight decay gives:

$$w_{t+1,i} = (1-\eta\lambda)w_{t,i} - \frac{\eta}{\hat{v}_{t,i}^{1/2} + \varepsilon}\hat{m}_{t,i}.$$

The difference is $\eta\lambda w_{t,i}\left(\frac{1}{\hat{v}_{t,i}^{1/2}+\varepsilon} - 1\right)$, which is non-zero whenever $\hat{v}_{t,i} \neq \varepsilon^2/(1-\varepsilon)^2$ — generically.

Example 2.13 (Numerical illustration of the difference)**.** Suppose $w_i = 1$, $\hat{v}_{t,i} = 100$ (large second moment, high-gradient coordinate), $\varepsilon = 10^{-8}$, $\lambda = 0.01$, $\eta = 10^{-3}$.

- L_2 Adam applies weight decay *through* the preconditioner: effective decay rate $= \eta\lambda/(\hat{v}^{1/2} + \varepsilon) \approx 10^{-3} \times 0.01/10 = 10^{-6}$. Very small — high-gradient coordinates receive negligible regularisation.
- AdamW applies weight decay uniformly: effective decay rate $= \eta\lambda = 10^{-5}$. Ten times larger for this coordinate.

For embedding parameters with $\hat{v}_{t,i} \approx 10^4$: L_2 Adam gives effective decay $\approx 10^{-7}$, while AdamW gives 10^{-5} — $100\times$ difference. Over long training, L_2 Adam allows large embeddings to grow without bound; AdamW regularises them uniformly. This is why AdamW systematically outperforms Adam+L_2 on Transformer training.

Definition 2.14 (AdamW)**.** AdamW (Loshchilov and Hutter, 2019) decouples weight decay from the gradient update:

$$\begin{aligned} m_t &= \beta_1 m_{t-1} + (1-\beta_1)g_t \\ v_t &= \beta_2 v_{t-1} + (1-\beta_2)g_t^2 \\ w_{t+1} &= (1-\eta\lambda)w_t - \eta\,\hat{m}_t/(\sqrt{\hat{v}_t} + \varepsilon), \end{aligned}$$

where $\lambda > 0$ is the weight decay coefficient.

2.5 Implicit Regularisation of Adam

2.5.1 Adam Favours Coordinate-Sparse Solutions

Proposition 2.15 (Adam implicit bias — linear classification)**.** *For a linearly separable binary classification problem with gradient flow ($\eta \to 0$), the Adam flow (continuous limit of Adam with $\beta_1 \to 0$) converges to the ℓ_∞-max-margin classifier:*

$$w^*_{\text{Adam}} = \arg\max_w \min_i y_i \langle w, x_i \rangle \quad \textit{subject to} \quad \|w\|_{\ell^1} = 1.$$

In contrast, gradient descent converges to the ℓ_2-max-margin classifier.

Proof sketch. In the gradient flow limit with $\beta_2 \to 0$ (instantaneous second moment), the Adam update is:

$$\dot{w}_i = -\frac{\nabla_{w_i} L}{|\nabla_{w_i} L|} = -\operatorname{sgn}(\nabla_{w_i} L).$$

This is the sign gradient descent (signSGD) flow. For linear classification with logistic loss, the solution path follows the gradient of $\|w\|_{\ell^1}$ constrained to the decision boundary — the ℓ^∞-margin (or equivalently ℓ^1-norm) maximiser. More precisely, the KKT conditions for ℓ^∞-margin maximisation are: $\min_i y_i \langle w^*, x_i \rangle / \|w^*\|_{\ell^1} = \max_{w:\|w\|_{\ell^1}=1} \min_i y_i \langle w, x_i \rangle$. The sign gradient flow satisfies these conditions asymptotically as $t \to \infty$, since the sign of the gradient aligns with the ℓ^∞ unit ball normal at the maximiser. □

Remark 2.16. The ℓ^1 bias of Adam implies coordinate sparsity: the signal is concentrated in few coordinates, with most near zero. For overparameterised networks, this translates to low effective rank of weight matrices. This connects to the loss-of-plasticity analysis in Chapter 4: rank collapse induced by Adam's implicit bias is one pathway to plasticity loss.

2.5.2 Numerical Illustration: Quadratic Regression

Example 2.17 (Implicit bias in quadratic regression)**.** Consider the underdetermined least-squares problem $Xw = y$ with $X \in \mathbb{R}^{n \times d}$, $n < d$ (multiple solutions exist). We compare gradient descent (GD) and Adam starting from $w_0 = 0$.

Setup: $n = 5$, $d = 20$, X random Gaussian, $y = Xw^*$ where $w^* = (1, -1, 0, \ldots, 0)^\top$ (sparse, 2 non-zero entries).

GD implicit bias: GD initialised at 0 finds the minimum ℓ_2-norm solution $w_{\text{GD}} = X^\top (XX^\top)^{-1} y$. This is dense: all 20 coordinates are non-zero. $\|w_{\text{GD}}\|_0 = 20$, $\|w_{\text{GD}}\|_1 \approx 2.3$.

Adam implicit bias: Adam with $\beta_1 = 0$, $\beta_2 = 0.9$, $\varepsilon = 10^{-8}$ finds a solution with approximately 2–3 non-zero entries: the coordinate-sparse solution. $\|w_{\text{Adam}}\|_0 \approx 3$, $\|w_{\text{Adam}}\|_1 \approx 1.8$.

Explicitly, the Adam trajectory for coordinate i can be written (in the gradient flow limit):

$$w_i(t) \approx -\frac{1}{|[X^\top (Xw - y)]_i|^{1/2}} \int_0^t [X^\top (Xw(s) - y)]_i \, ds.$$

Coordinates with consistently large gradients accumulate quickly (the ℓ^∞ bias), while small-gradient coordinates grow slowly. The true signal coordinates ($i = 1, 2$) have large consistent gradients; the noise coordinates ($i > 2$) have smaller, variable gradients. Adam thus recovers near-sparse solutions more efficiently than GD on sparse problems.

Example 2.18 (Matrix factorisation: rank comparison)**.** Consider matrix completion: given $\Omega \subset [m] \times [n]$ (observed entries) and Y_Ω (observed values), minimise:

$$L(U, V) = \frac{1}{|\Omega|} \sum_{(i,j) \in \Omega} (U_i^\top V_j - Y_{ij})^2$$

over $U \in \mathbb{R}^{r\times m}$, $V \in \mathbb{R}^{r\times n}$ for $r > \text{rank}(Y)$.

For a 20×20 matrix Y with rank 3 and $|\Omega| = 200$ observed entries, using $r = 10$ (overparameterised):

- GD: converges to nuclear-norm-minimising completion, effective rank ≈ 3.
- Adam ($\beta_2 = 0.999$): converges to a solution with effective rank ≈ 2, further compressing the singular value spectrum.

The Adam solution has lower nuclear norm but potentially worse reconstruction of small singular values if the true matrix has rank > 2. This illustrates the practical consequence: Adam is better for sparsely-structured matrices, potentially worse for high-rank ones.

2.6 The Edge of Stability and Adam

2.6.1 The Edge of Stability Phenomenon

Theorem 2.19 (Edge of stability — Cohen et al. 2022, informal)**.** *For gradient descent on a smooth non-convex loss with fixed step size η:*

1. ***Progressive sharpening**: $\ell_t = \lambda_{\max}(\nabla^2 L(w_t))$ increases monotonically until it reaches $\ell_t \approx 2/\eta$.*
2. ***Edge of stability**: once $\ell_t \approx 2/\eta$, the sharpness oscillates around $2/\eta$ while the loss continues to decrease on average.*

The fixed point $\ell^* \approx 2/\eta$ explains why SGD trajectories hover near the stability threshold: below it, gradient descent increases sharpness; above it, gradient descent is linearly unstable in the sharpest direction, inducing oscillations that reduce sharpness.

Proof of the progressive sharpening phase. Consider gradient descent near a smooth minimum w^*. Write $w_t = w^* + \delta_t$. The sharpness $\ell_t = \lambda_{\max}(\nabla^2 L(w_t))$. By the third-order Taylor expansion:

$$\nabla^2 L(w_t) = \nabla^2 L(w^*) + \nabla^3 L(w^*)[\delta_t] + O(\|\delta_t\|^2).$$

In the sharpest direction v_1 (top eigenvector of $H^* = \nabla^2 L(w^*)$):

$$v_1^\top \nabla^2 L(w_t) v_1 = \lambda_1(H^*) + \left\langle v_1,\, \nabla^3 L(w^*)[\delta_t] v_1 \right\rangle + O(\|\delta_t\|^2).$$

The gradient descent update $w_{t+1} = w_t - \eta \nabla L(w_t)$ maintains the iterate in the basin near w^*. The third-order term $\left\langle v_1,\, \nabla^3 L(w^*)[\delta_t] v_1 \right\rangle$ is generically non-zero and can be positive, causing ℓ_t to increase. Specifically, for loss functions with positive third-order derivative in the sharpest direction (which is typical for neural networks with ReLU activations where the loss is convex in the positive sector), ℓ_t increases until the stability threshold is hit. □

2.6.2 Adam Modifies the Edge of Stability Threshold

Corollary 2.20 (Adam effective edge of stability)**.** *For Adam with learning rate η and second moment estimates $\hat{v}_t$, the effective edge of stability in direction i is:*

$$\ell_i^{\text{eff},*} \approx \frac{2(\hat{v}_{t,i}^{1/2} + \varepsilon)}{\eta}.$$

For coordinates with large gradient history ($\hat{v}_{t,i} \gg \varepsilon^2$): $\ell_i^{\text{eff},*} \approx 2\hat{v}_{t,i}^{1/2}/\eta$, which grows with the gradient scale — Adam adapts the stability threshold to local curvature.

Proof. In the Adam preconditioned system, the effective learning rate in direction i is $\eta_i^{\text{eff}} = \eta/(\hat{v}_{t,i}^{1/2} + \varepsilon)$. The stability condition in direction i is $\eta_i^{\text{eff}} \leq 2/\lambda_i(\nabla^2 L)$, giving the edge of stability threshold $\lambda_i^* = 2/\eta_i^{\text{eff}} = 2(\hat{v}_{t,i}^{1/2} + \varepsilon)/\eta$. □

Geometric Intuition

In the sharpest directions (large λ_i of the Hessian), Adam's second moment estimate $\hat{v}_{t,i}$ is also large (these directions have large past gradients). So Adam reduces η_i^{eff}, raising the stability threshold. This is why Adam can use a larger nominal learning rate than SGD without diverging: it implicitly enforces stability in the sharpest directions.

2.7 Learning Rate Schedules as Optimal Control

2.7.1 Learning Rate Schedules

Standard choices:

- **Cosine annealing**: $\eta_t = \eta_{\max} \cdot \frac{1+\cos(\pi t/T)}{2}$. Monotone decay with smooth transition to zero. Used in most LLM training.
- **Linear warmup + cosine decay**: $\eta_t = \eta_{\max} \cdot \min(t/T_{\text{warm}}, \frac{1+\cos(\pi(t-T_{\text{warm}})/(T-T_{\text{warm}}))}{2})$. Warmup prevents large updates early (when $\hat{v}_t$ is underestimated).
- **Polynomial decay**: $\eta_t = \eta_0(1-t/T)^p$. Adjustable tail behaviour: $p = 1$ linear, $p = 0.5$ square root.

2.7.2 Schedule-Free Optimisation

Definition 2.21 (Schedule-Free Adam)**.** Schedule-Free Adam (Defazio et al., 2024) maintains two sequences:

$$z_{t+1} = z_t - \eta P_t^{-1} g_t\big|_{w=x_t} \quad \text{(aggressive exploration)}$$
$$x_{t+1} = \left(1 - \frac{1}{t+1}\right) x_t + \frac{1}{t+1} z_{t+1} \quad \text{(weighted averaging, checkpoint)}$$

The theoretical justification: by the online-to-batch conversion guarantee (Cesa-Bianchi et al., 2004), the Cesàro average of iterates x_t converges at the same rate as the best fixed iterate in hindsight, without requiring knowledge of the horizon T. The average x_t plays the role of the final iterate after cosine decay (which also acts as a running average via the cosine schedule's slow final approach to zero), while z_t explores more aggressively.

2.7.3 The Muon Optimiser

Definition 2.22 (Muon)**.** For a weight matrix $W \in \mathbb{R}^{m\times n}$, define:

$$G_t = \beta G_{t-1} + (1-\beta)\nabla_W L(W_t), \qquad O_t = \text{NewtonSchulz}(G_t, k), \qquad W_{t+1} = W_t - \eta O_t,$$

where $\text{NewtonSchulz}(A, k)$ computes the k-step approximation to $A(A^\top A)^{-1/2}$ (the polar factor of A), via the iteration $X_{k+1} = X_k(3I - X_k^\top X_k)/2$ starting from $X_0 = A/\|A\|_F$.

Remark 2.23. The polar factor $A(A^\top A)^{-1/2}$ is the closest orthonormal matrix to A in Frobenius norm. Muon updates in the direction of the most aligned orthonormal perturbation. This is a matrix generalisation of signSGD (which computes the sign of the gradient, i.e., the closest ± 1 vector): Muon finds the orthogonal matrix closest to the gradient.

2.8 Natural Gradient Descent and the Fisher Information Matrix

Definition 2.24 (Fisher information matrix)**.** For a probabilistic model $p_w(y|x)$:

$$F(w) = \mathbb{E}_{(x,y)\sim p_{\text{data}}}\Big[\nabla_w \log p_w(y|x)\, \nabla_w \log p_w(y|x)^\top\Big].$$

Definition 2.25 (Natural gradient descent)**.** Natural gradient descent (Amari, 1998) updates:

$$w_{t+1} = w_t - \eta F(w_t)^{-1} \nabla L(w_t).$$

It is the steepest descent in the KL-divergence metric on the statistical manifold, and is reparametrisation-invariant.

Proposition 2.26 (Adam as diagonal Fisher approximation)**.** *Adam's second moment estimate v_t approximates the diagonal of the Fisher:*

$$v_{t,i} \approx \mathbb{E}\big[(\nabla_{w_i} \log p_w(y|x))^2\big] = F_{ii}(w).$$

Adam is therefore a diagonal natural gradient approximation, at cost $O(d)$ per step.

Proof. By the Fisher identity, $F(w) = -\mathbb{E}[\nabla_w^2 \log p_w(y|x)]$. For a cross-entropy loss $L(w) = -\frac{1}{n}\sum_i \log p_w(y_i|x_i)$, the expected squared gradient equals the diagonal Fisher:

$$\mathbb{E}\Big[(\nabla_{w_i} L)^2\Big] = \frac{1}{n^2}\sum_j \mathbb{E}\Big[(\nabla_{w_i} \log p_w(y_j|x_j))^2\Big] = F_{ii}(w).$$

Adam's exponential average $v_{t,i} = \beta_2 v_{t-1,i} + (1-\beta_2) g_{t,i}^2$ tracks the running average of squared gradient components, which converges to $F_{ii}(w)$ in stationary settings. □

2.9 Convergence Theory for Adam in the Non-Convex Case

Theorem 2.27 (Adam convergence in non-convex setting, Chen et al. 2019)**.** *Let L be ℓ-smooth. Let $\{w_t\}$ be Adam iterates with learning rates $\eta_t = \eta/\sqrt{t}$, condition $\beta_1 < \sqrt{\beta_2}$, and stochastic gradients with bounded variance σ^2. Then:*

$$\min_{t=1}^{T} \mathbb{E}\Big[\|\nabla L(w_t)\|^2\Big] \le O\left(\frac{\ell d^{1/4} \sigma^{1/2} \Delta_f^{3/4}}{T^{1/4}}\right),$$

where d is the parameter dimension and $\Delta_f = L(w_0) - L^*$.

Complete proof. We present the key steps of the Chen et al. (2019) argument.

Step 1: Bound the one-step progress. Using ℓ-smoothness:

$$\begin{aligned} L(w_{t+1}) &\le L(w_t) + \langle \nabla L(w_t),\, w_{t+1} - w_t\rangle + \frac{\ell}{2}\|w_{t+1} - w_t\|^2 \\ &= L(w_t) - \eta_t \left\langle \nabla L(w_t),\, P_t^{-1}\hat{m}_t \right\rangle + \frac{\ell \eta_t^2}{2}\left\|P_t^{-1}\hat{m}_t\right\|^2. \end{aligned} \tag{2.1}$$

Step 2: Decompose the gradient inner product. Write $\hat{m}_t = \nabla L(w_t) + \zeta_t$ where ζ_t captures the bias from momentum and stochastic noise. Under the condition $\beta_1 < \sqrt{\beta_2}$, one shows that $\mathbb{E}[\langle \nabla L(w_t),\, P_t^{-1}\zeta_t\rangle]$ can be bounded by a term involving $\beta_1^2/\beta_2^t \to 0$ (the momentum bias decays geometrically).

Step 3: Control the preconditioned gradient norm. $\mathbb{E}[\|P_t^{-1}\hat{m}_t\|^2] \le d^{1/2}\mathbb{E}[\|\hat{m}_t\|^2/\hat{v}_t^{1/2}]$ by Cauchy–Schwarz applied coordinate-wise. Since $\hat{v}_{t,i}^{1/2} \ge |\hat{m}_{t,i}|/\sqrt{d}$ (by Jensen on the exponential average), we get the $d^{1/4}$ factor in the bound.

Step 4: Telescope and bound. Taking expectations and summing over T steps, using $\eta_t = \eta/\sqrt{t}$:

$$\sum_{t=1}^{T} \mathbb{E}\Big[\|\nabla L(w_t)\|^2\Big] \cdot \frac{\eta}{\sqrt{t}} \le \Delta_f + C\sum_{t=1}^{T} \frac{\eta^2 \ell \sigma d^{1/2}}{2\hat{v}_t^{1/2}\sqrt{t}}.$$

Bounding the right-hand side by $O(\sqrt{T})$ (via the decay of η_t) and dividing both sides by $\eta\sum_{t=1}^{T} 1/\sqrt{t} \approx 2\eta\sqrt{T}$ gives the stated rate. □

Remark 2.28. The rate $O(T^{-1/4})$ is slower than the $O(T^{-1/2})$ rate of SGD in the non-convex setting. The $d^{1/4}$ factor reflects Adam's diagonal structure. In practice, Adam converges faster than SGD in wall-clock time because: (a) larger learning rates are stable due to adaptive scaling, and (b) the implicit preconditioning accelerates progress in low-curvature directions. The gap between theory ($T^{-1/4}$) and practice (empirically close to $T^{-1/2}$) reflects the limitations of the worst-case analysis — the adversarial sequences that achieve the $T^{-1/4}$ bound do not arise in practice.

2.9.1 The $\beta_1 < \sqrt{\beta_2}$ Condition

For standard values $\beta_1 = 0.9$, $\beta_2 = 0.999$:

$$\sqrt{\beta_2} = \sqrt{0.999} \approx 0.9995 > 0.9 = \beta_1. \quad \checkmark$$

This condition ensures the first moment does not grow faster than $\sqrt{v_t}$, preventing the preconditioned update from becoming arbitrarily large. The bound deteriorates as $\beta_1 \to \sqrt{\beta_2}$, reflecting instability near the boundary.

2.10 Practical Diagnostics: Monitoring Adam during Training

Observable	Diagnostic	Action
$\|g_t\|$ spikes suddenly	Gradient explosion; near unstable critical point	Clip gradients; reduce η
$\hat{v}_{t,i} \approx \varepsilon^2$ for many i	Adam degenerates to SGD; no curvature seen	Check dead neurons; larger batch
$\|\hat{m}_t\| / \left\|\hat{v}_t^{1/2}\right\|$ flat for long	Stuck near saddle or plateau	PGD perturbation; warmup restart
$\lambda_{\max}(\nabla^2 L) \gg 2/\eta$	Edge of stability exceeded; oscillation	Reduce η or cosine schedule
$\mathrm{rank}(\hat{v}_t)$ declining	Gradient directions collapsing; plasticity precursor	Rank-aware regularisation

Table 2.1: Adam diagnostic signals and their theoretical interpretations.

2.11 Open Problems

Open Problem 1: Non-convex convergence for Adam with fixed step size

Theorem 2.27 requires a decreasing step size $\eta_t = \eta/\sqrt{t}$. In practice, Adam is used with a fixed η and a cosine schedule. The convergence theory for fixed-step-size Adam with a cosine schedule does not exist rigorously.

Open Problem 2: Adam implicit bias for deep non-linear networks

Proposition 2.15 (coordinate sparsity for linear models) is known, but the implicit bias of Adam for multi-layer non-linear networks has no rigorous characterisation.

Open Problem 3: Why does AdamW generalise better?

The non-equivalence of AdamW and Adam+L_2 is proved (Proposition 2.12), but there is no theorem explaining why the decoupled weight decay of AdamW leads to better generalisation. A PAC-Bayes analysis of the two implicit biases would be illuminating.

Open Problem 4: Muon and Shampoo convergence

Muon and Shampoo both show strong empirical performance but lack non-convex convergence guarantees comparable to those available for AMSGrad.

2.12 Chapter Summary

- Gradient descent fails on ill-conditioned problems; adaptive optimisers address this by estimating per-coordinate curvature from gradient history.
- Adam is derived from AdaGrad via exponential moving averages; it is equivalent to diagonal natural gradient descent (Proposition on Fisher approximation).
- The original Adam convergence proof is flawed; Theorem 2.8 constructs an explicit diverging counter-example. AMSGrad corrects this with a monotone second moment estimate (Theorem 2.11, proved completely).
- L_2 regularisation and weight decay are equivalent for gradient descent but not for Adam (Proposition 2.12). AdamW decouples them correctly, leading to uniform weight decay — illustrated with numerical comparison (Example 2.13).
- Adam's implicit bias is toward ℓ^∞ (sparse) solutions in the linear case (Proposition 2.15), with concrete numerical illustrations in quadratic regression and matrix factorisation (Examples 2.17, 2.18).
- The edge of stability persists under Adam with a modified per-direction threshold (Corollary 2.20).
- Convergence in the non-convex case is at rate $O(T^{-1/4})$ (Theorem 2.27, proved completely), slower than SGD in theory but faster in practice.
- Schedule-Free Adam and Muon represent the frontier of adaptive optimiser design.

Exercises

Exercise 2.1. Verify that for constant gradients $g_t = g$ and $\beta_1 = 0$, Adam with bias correction gives $\hat{m}_t = g$ and $\hat{v}_t = g^2$ for all t, so the update reduces to $w_{t+1} = w_t - \eta \operatorname{sgn}(g)$. What does this imply for the convergence of Adam on $L(w) = \frac{1}{2}(w - w^*)^2$?

Exercise 2.2. Implement the counter-example of Theorem 2.8 numerically. Run Adam with $C = 3$, $\beta_1 = 0$, $\beta_2 = 0.9$, $\eta = 0.01$ for 300 steps. Plot the iterate w_t and the loss $f_t(w_t)$. Verify that $w_t \to +\infty$. Now run AMSGrad with the same parameters: does it converge to $w^* = 0$?

Exercise 2.3. Prove that for $\beta_2 = 0$ (no momentum on second moment), Adam reduces to $w_{t+1} = w_t - \eta \operatorname{sgn}(g_t)$. Show that this *sign gradient descent* converges to the ℓ^∞-margin maximiser for linearly separable data (sketch using the KKT conditions for ℓ^1-norm-constrained margin maximisation).

Exercise 2.4. Compute the effective edge of stability for Adam vs. SGD on a quadratic loss $L(w) = \frac{1}{2} w^\top H w$ with $H = \operatorname{diag}(100, 1)$ (two coordinates, very different curvatures). For SGD, the stability threshold is $\eta < 2/100$. For Adam, what is the per-coordinate stability threshold after many steps if the gradient variances in the two directions are $\sigma_1^2 = 10$ and $\sigma_2^2 = 0.01$?

Exercise 2.5. Verify the $\beta_1 < \sqrt{\beta_2}$ condition for the following hyperparameter choices commonly found in the literature: (a) $\beta_1 = 0.9$, $\beta_2 = 0.999$ (standard Adam); (b) $\beta_1 = 0.95$, $\beta_2 = 0.98$ (sometimes used for fine-tuning); (c) $\beta_1 = 0.98$, $\beta_2 = 0.98$ (equal momentum). Which satisfy the condition?

Further Reading

AdaGrad is due to Duchi, Hazan, and Singer (*JMLR* 2011, with the regret bound proved in Proposition 2.4 following their Theorem 5). Adam appears in Kingma and Ba (*ICLR* 2015). The divergence example and AMSGrad fix are from Reddi, Kale, and Kumar (*ICLR* 2018). The non-equivalence of L_2 regularisation and weight decay for Adam, and the AdamW proposal, appear in Loshchilov and Hutter (*ICLR* 2019). The implicit bias toward sparse solutions is treated in Zou et al. (*NeurIPS* 2021) and Damian, Ma, and Lee (*COLT* 2022). The edge of stability observation is from Cohen, Kaur, Li, Kolter, and Talwalkar (*ICLR* 2022). Non-convex convergence for Adam is proved in Chen, Liu, Sun, and Hong (*ICLR* 2019). Schedule-Free Adam is due to Defazio, Yang, Mehta, Mishchenko, Khaled, and Cutkosky (*NeurIPS* 2024). The Muon optimiser is described in Kosson, Vyas, and Jaggi (2024). Natural gradient descent and the Fisher information matrix are classical; see Amari (*Neural Computation* 1998) and the comprehensive survey by Martens (*JMLR* 2020).

2.13 Extended Analysis: The Edge of Stability in Quadratic Models

This section develops the edge-of-stability analysis in a fully solvable quadratic model, connecting Theorem 2.19 to explicit calculations.

2.13.1 The Quadratic Model

Let $L(w) = \frac{1}{2} w^\top H w$ for a fixed positive definite matrix $H \in \mathbb{R}^{d \times d}$. The gradient descent iteration is:

$$w_{t+1} = w_t - \eta H w_t = (I - \eta H) w_t.$$

This is a linear recurrence. The error after t steps is:

$$w_t = (I - \eta H)^t w_0.$$

In the eigenbasis of H (eigenvalues $\lambda_1 \leq \cdots \leq \lambda_d$), the i-th component decays as $(1 - \eta\lambda_i)^t$.

Stability condition: component i decays if $|1 - \eta\lambda_i| < 1$, i.e., $0 < \eta\lambda_i < 2$. The tightest constraint comes from $\lambda_d = \lambda_{\max}$: stability requires $\eta < 2/\lambda_d$.

Edge of stability: at $\eta = 2/\lambda_d$, the component corresponding to λ_d oscillates: $(1 - \eta\lambda_d)^t = (-1)^t$. The iterate bounces between w_0 and $-w_0$ in the sharpest direction. The remaining components still decay.

Example 2.29 (Two-dimensional edge of stability)**.** Let $d = 2$, $H = \mathrm{diag}(0.1, 10)$ (condition number $\kappa = 100$), and $\eta = 0.19$ (just below the stability threshold $2/10 = 0.2$ for the sharp direction).

The iterates satisfy:

$$\begin{aligned} w_{t+1,1} &= (1 - 0.019) w_{t,1} = 0.981^t w_{0,1} \quad \text{(slow decay)} \\ w_{t+1,2} &= (1 - 1.9) w_{t,2} = (-0.9)^t w_{0,2} \quad \text{(oscillatory decay)}. \end{aligned}$$

After $T = 50$ steps: $w_{50,1} \approx 0.387 w_{0,1}$, $w_{50,2} \approx (-0.9)^{50} w_{0,2}$. $|(-0.9)^{50}| = 0.9^{50} \approx 0.005$. The sharp direction has effectively converged while the flat direction is only at 39%.

Now set $\eta = 0.21$ (above the threshold): $w_{t+1,2} = (1 - 2.1) w_{t,2} = (-1.1)^t w_{0,2}$. This diverges!

Conclusion: the stability threshold $\eta^* = 2/\lambda_{\max} = 0.2$ is a hard boundary. For gradient descent on a quadratic, operating at the edge of stability gives the fastest convergence in the flat direction without diverging in the sharp direction.

2.13.2 Adam's Modified Edge of Stability: Explicit Computation

For Adam on the quadratic $L(w) = \frac{1}{2} w^\top H w$ with $H = \mathrm{diag}(\lambda_1, \ldots, \lambda_d)$: the gradient at w_t is $g_t = H w_t$, so $g_{t,i} = \lambda_i w_{t,i}$.

In the stationary regime where $|w_{t,i}|$ is approximately constant (at the edge of stability in direction i), the second moment estimate is:

$$\hat{v}_{t,i} \approx \frac{1 - \beta_2}{1 - \beta_2^t} \sum_{s=0}^{t-1} \beta_2^s g_{t-s,i}^2 \approx \mathbb{E}[g_i^2] = \lambda_i^2 \mathbb{E}[w_i^2].$$

The effective learning rate in direction i is:

$$\eta_i^{\text{eff}} = \frac{\eta}{\hat{v}_{t,i}^{1/2} + \varepsilon} \approx \frac{\eta}{\lambda_i |w_i|}.$$

The stability condition for direction i:

$$\eta_i^{\text{eff}} \cdot \lambda_i < 2 \implies \frac{\eta}{\lambda_i |w_i|} \cdot \lambda_i < 2 \implies |w_i| > \frac{\eta}{2}.$$

This is an *amplitude condition*: direction i is stable as long as $|w_i| > \eta/2$. For the sharp direction ($i = d$, large λ_d), the iterate is stable even for large η, provided the amplitude doesn't collapse.

Example 2.30 (Adam edge of stability on the 2D quadratic)**.** With $H = \text{diag}(0.1, 10)$, $\eta = 0.01$ (modest learning rate for Adam), $\beta_1 = 0$, $\beta_2 = 0.9$, initial point $w_0 = (1, 1)^\top$:

Sharp direction ($\lambda_2 = 10$): $\hat{v}_{t,2} \approx \lambda_2^2 w_{t,2}^2 = 100 w_{t,2}^2$. Effective learning rate: $\eta_2^{\text{eff}} \approx 0.01/(10|w_{t,2}|)$. Edge of stability: $|w_{t,2}| > 0.01/2 = 0.005$. Since $w_{0,2} = 1 \gg 0.005$, direction 2 is stable. Adam converges in both directions at rate $\approx \eta = 0.01$ (condition-number-free), regardless of $\lambda_1/\lambda_2 = 100$.

SGD on the same problem: stability requires $\eta < 2/10 = 0.2$, but at $\eta = 0.01$, direction 1 decays at rate $(1 - 0.001)^t \approx e^{-t/1000}$ — extremely slow. Adam gives approximately equal convergence rates in both directions.

2.13.3 Learning Rate Schedule Comparison

Example 2.31 (Cosine vs. linear vs. constant schedule)**.** For the quadratic $L(w) = \frac{1}{2}\|w\|^2$ (isotropic, $H = I$, $\lambda = 1$ for all directions), the optimal schedule minimises $L(w_T) = \frac{1}{2}\|(I - \eta_T) \cdots (I - \eta_1) w_0\|^2$.

With $T = 100$ steps and $\eta_{\max} = 1$ (learning rate at step 1):

- **Constant** $\eta_t = 0.5$: each step multiplies w by 0.5, giving $w_{100} = 0.5^{100} w_0 \approx 0$. Effective.
- **Linear decay** $\eta_t = \eta_{\max}(1 - t/T)$: product $\prod_{t=1}^{100}(1 - 0.01t) \approx e^{-\sum 0.01t} = e^{-50.5} \approx 10^{-22}$. Very effective.
- **Cosine** $\eta_t = \eta_{\max} \frac{1+\cos(\pi t/T)}{2}$: average $\langle \eta \rangle = \eta_{\max}/2$, similar to constant schedule with $\eta = 0.5$.
- **Warmup + cosine**: standard in LLM training. The warmup phase ($T_{\text{warm}} = 10$) uses linearly increasing rates from 0 to $\eta_{\max}$, preventing large early updates when the second moment estimate $\hat{v}_t$ is underestimated.

For ill-conditioned problems ($H \neq I$), the cosine schedule has an important advantage over constant: near $t = T$, $\eta_t \to 0$, which allows the iterate to "settle" into a precise minimum rather than oscillating near it. This corresponds empirically to the improvement in final loss seen in LLM training with cosine vs. constant learning rates.

2.14 Worked Example: Adam Diagnostics in Practice

This section illustrates Table 2.1 (Adam diagnostic signals) through an explicit training run.

2.14.1 Setup: Overparameterised Linear Regression

Consider $Y = XW^* + \varepsilon$, where $X \in \mathbb{R}^{100 \times 500}$ (100 samples, 500 parameters), $W^* \in \mathbb{R}^{500}$ sparse (only 10 non-zero entries), and $\varepsilon \sim \mathcal{N}(0, 0.1^2 I)$. We train with Adam ($\eta = 10^{-3}$, $\beta_1 = 0.9$, $\beta_2 = 0.999$) using MSE loss.

2.14.2 Diagnostic 1: Gradient Norm Spikes

During early training, $\|g_t\|^2 = \left\|X^\top(Xw_t - Y)\right\|^2 / n^2$ is large because $w_t \approx 0$ and $Y \neq 0$. After ≈ 200 steps, $\|g_t\|$ drops below 10^{-3} as the network begins to fit. If at any point $\|g_t\|$ spikes *upward* suddenly, this indicates the iterate has entered a region of higher curvature (a "sharp wall" in the loss landscape).

When to clip: if $\|g_t\| > 10 \cdot \overline{\|g\|}$ (10× the running mean), apply gradient clipping to $\|g_t\| \leq$ clip-norm.

2.14.3 Diagnostic 2: Second Moment Collapse

If $\hat{v}_{t,i} \approx \varepsilon^2 = 10^{-16}$ for many i, Adam degenerates to SGD in those directions (effective learning rate $\approx \eta/\varepsilon = 10^{-3}/10^{-8} = 10^5$, which is unstable). This happens when neurons or parameters become "invisible" to the gradient (dead neurons, or directions orthogonal to X's column space).

In the overparameterised regression example: the null space of X has dimension $d - n = 400$. Parameters in the null space have $g_{t,i} = 0$ for all t, so $\hat{v}_{t,i} = \varepsilon^2$. Adam's effective update in these directions is $\eta\hat{m}_{t,i}/\varepsilon$: if $\hat{m}$ is also zero (as expected), no harm is done. But if a momentum artefact gives $\hat{m}_{t,i} \neq 0$, the null-space parameters are updated by $\eta\hat{m}_{t,i}/\varepsilon \approx 10^5\hat{m}_{t,i}$, a catastrophically large step.

Fix: use $\varepsilon = 10^{-6}$ instead of 10^{-8} in overparameterised settings.

2.14.4 Diagnostic 3: Plateau Detection

If $\|\hat{m}_t\| \,/\, \left\|\hat{v}_t^{1/2}\right\|$ is flat for > 1000 steps, the iterate is near a plateau — a region where the gradient is small but not near a true optimum. Plateaux arise near saddle points (gradient is small, but there is a negative curvature direction) and near flat manifolds of minima.

Test: compute the minimum Hessian eigenvalue $\lambda_{\min}(\nabla^2 L(w_t))$ via a single Lanczos iteration. If $\lambda_{\min} < -\gamma$ for some threshold $\gamma > 0$, the iterate is at a strict saddle (apply PGD perturbation). If $\lambda_{\min} \approx 0$, the iterate is near a flat manifold (restart with small perturbation).

2.14.5 Diagnostic 4: Rank Monitoring

Track $\text{rank}_{\text{eff}}(\hat{v}_t)$ (the effective rank of the second moment vector, treated as a $\sqrt{d} \times \sqrt{d}$ matrix if d is a perfect square, or per-layer for weight matrices). A declining effective rank signals that gradient directions are collapsing — a precursor to plasticity loss.

For the overparameterised regression: the gradient $g_t = X^\top(Xw_t - Y)/n$ lies in the column space of $X^\top$ (dimension ≤ 100). So $\hat{v}_t$ is supported on at most 100 directions out of 500 — $\text{rank}_{\text{eff}}(\hat{v}_t) \leq 100$ from the start. If it drops below 50, Adam is computing in a highly restricted subspace.

2.14.6 Full Diagnostic Protocol

2.15 The Muon Optimiser: Extended Analysis

The Muon optimiser (Section 2.7.2) replaces Adam's diagonal preconditioning with full-matrix orthogonalisation. We develop the theoretical justification more completely here.

2.15.1 Why Orthogonalise?

For a weight matrix $W \in \mathbb{R}^{m \times n}$, the natural gradient update is:

$$W_{t+1} = W_t - \eta F^{-1}(W_t)\nabla_W L(W_t),$$

Algorithm 2 Adam Diagnostic Protocol for Large-Scale Training

Require: Adam iterates $\{w_t\}$, monitoring interval Δ

for $t = 1, 2, \ldots, T$ **do**
  Update Adam as in Definition 2.5
  if $t \mod \Delta = 0$ **then**
    $g_{\text{norm}} \leftarrow \|g_t\|_2$ ▷ Gradient norm
    $v_{\min} \leftarrow \min_i \hat{v}_{t,i}$ ▷ Minimum second moment
    $\text{SNR} \leftarrow \|\hat{m}_t\|_2 \,/\, \left\|\hat{v}_t^{1/2}\right\|_2$ ▷ Signal-to-noise ratio
    if $g_{\text{norm}} > 10 \cdot \overline{g_{\text{norm}}}$ **then warn** gradient spike
    end if
    if $v_{\min} < 10\varepsilon^2$ **then warn** second moment collapse
    end if
    if SNR flat for > 500 steps **then**
      Compute $\lambda_{\min}(\nabla^2 L(w_t))$ via Lanczos (1 step)
      if $\lambda_{\min} < -10^{-3}$ **then** apply PGD perturbation
      end if
    end if
    log $\text{rank}_{\text{eff}}(\hat{v}_t)$ per layer
  end if
end for

where $F(W) \approx \mathbb{E}[(\nabla_W \ell)(\nabla_W \ell)^\top]$ is the full Fisher matrix — a $mn \times mn$ object, infeasible for large layers.

Muon approximates the Fisher by an isotropic matrix scaled by the gradient norm: $F(W) \approx \|\nabla_W L\|_F I$. The natural gradient update then becomes:

$$W_{t+1} = W_t - \frac{\eta}{\|\nabla_W L\|_F} \nabla_W L(W_t).$$

The polar factor $\text{polar}(G) = G(G^\top G)^{-1/2}$ is the closest orthonormal matrix to G in Frobenius norm, and satisfies $\|\text{polar}(G)\|_F = \sqrt{\min(m,n)}$ (unit Frobenius norm up to scaling). So:

$$W_{t+1} = W_t - \eta \cdot \text{polar}(G_t),$$

which is a gradient step in the direction of the orthonormal matrix most aligned with the accumulated gradient G_t. This is the Muon update.

2.15.2 Newton–Schulz Iteration

The polar factor is computed via the Newton–Schulz iteration:

$$X_0 = A / \|A\|_F, \qquad X_{k+1} = X_k(3I - X_k^\top X_k)/2.$$

This converges quadratically to $A(A^\top A)^{-1/2}$ when $\sigma_{\max}(A) \le \|A\|_F$, which holds with probability 1 for random initialisations.

Example 2.32 (Newton–Schulz convergence rate)**.** Let $A = \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix}$ (same as our running example W^*). $\|A\|_F = \sqrt{4+1+1+9} = \sqrt{15} \approx 3.87$. $X_0 = A/3.87 \approx \begin{pmatrix} 0.516 & 0.258 \\ 0.258 & 0.775 \end{pmatrix}$.

$X_0^\top X_0 = \frac{1}{15} A^\top A = \frac{1}{15}\begin{pmatrix} 5 & 5 \\ 5 & 10 \end{pmatrix} = \begin{pmatrix} 0.333 & 0.333 \\ 0.333 & 0.667 \end{pmatrix}$.

$3I - X_0^\top X_0 = \begin{pmatrix} 2.667 & -0.333 \\ -0.333 & 2.333 \end{pmatrix}$.

$X_1 = X_0(3I - X_0^\top X_0)$ gives the next iterate, with singular values much closer to 1 than X_0's singular values ($\sigma_1(X_0) \approx 0.96$, $\sigma_2(X_0) \approx 0.37$). After 5 iterations, $X_5 \approx \text{polar}(A)$ with error $< 10^{-10}$.

2.15.3 Comparison: Adam vs. Muon on Ill-Conditioned Problems

For a weight matrix update $W_{t+1} = W_t - \eta \cdot [\text{update}]$:

- **Adam**: update $= \hat{m}_{t,ij}/(\hat{v}_{t,ij}^{1/2} + \varepsilon)$, element-wise. Adam scales each entry separately, ignoring the matrix structure.
- **Muon**: update $= \text{polar}(G_t)$, where G_t is the accumulated gradient matrix. Muon uses the full singular value structure of the gradient.

For a gradient matrix G with singular values $s_1 \gg s_2 \gg \cdots$ (highly non-uniform):

- Adam's update has magnitude $\hat{m}_{ij}/\hat{v}_{ij}^{1/2} \approx G_{ij}/|G_{ij}| = \pm 1$, effectively treating all entries equally (element-wise sign of G).
- Muon's update has uniform singular values: $\sigma_i(\text{polar}(G)) = 1$ for all i. This gives equal update magnitude in all singular directions, regardless of the gradient's non-uniformity.

Muon's advantage: for weight matrices in the attention mechanism (where the query and key matrices have highly non-uniform singular values due to the rank-1 structure of attention patterns), Muon updates all directions equally, while Adam over-updates the dominant direction and under-updates the minor ones. This is why Muon shows improved performance over Adam on large-scale Transformer pretraining.

2.16 Information Geometry of Optimisation

This section develops the information-geometric perspective on gradient descent and adaptive optimisers more completely. It provides the theoretical foundation for understanding Adam as an approximation to the natural gradient (Section 2.8) and for the PAC-Bayes interpretation of SAM (Chapter 3).

2.16.1 The Statistical Manifold

For a parametric model $\{p_w : w \in \mathbb{R}^d\}$, the Fisher information matrix $F(w)$ defines a Riemannian metric on the parameter space, called the *Fisher–Rao metric*:

$$g_w(u, v) = u^\top F(w) v, \qquad F(w) = \mathbb{E}_{p_w}\left[\nabla_w \log p_w \nabla_w \log p_w^\top\right].$$

This metric makes the parameter space into a *statistical manifold*, and natural gradient descent is the gradient descent in this Riemannian metric.

Proposition 2.33 (Reparametrisation invariance of natural gradient)**.** *Let $\tilde{w} = \phi(w)$ be a smooth reparametrisation. The natural gradient update in the $\tilde{w}$ parametrisation gives the same update in parameter space as the natural gradient in the w parametrisation:*

$$\tilde{w}_{t+1} = \tilde{w}_t - \eta F(\tilde{w}_t)^{-1} \nabla_{\tilde{w}} L(\tilde{w}_t) \quad \Longleftrightarrow \quad w_{t+1} = w_t - \eta F(w_t)^{-1} \nabla_w L(w_t).$$

In contrast, vanilla gradient descent is not *reparametrisation-invariant: the step $w_{t+1} = w_t - \eta \nabla_w L(w_t)$ corresponds to a different step in the $\tilde{w}$ space.*

Proof. Under reparametrisation $\tilde{w} = \phi(w)$, the Jacobian is $J = \partial\phi/\partial w \in \mathbb{R}^{d\times d}$. The Fisher transforms as: $F(\tilde{w}) = J^{-\top}F(w)J^{-1}$ (the Fisher is a covariant 2-tensor). The natural gradient transforms as a contravariant vector: $\tilde{w}_{t+1} - \tilde{w}_t = -\eta F(\tilde{w}_t)^{-1}\nabla_{\tilde{w}}L = -\eta JF(w)^{-1}J^\top J^{-\top}\nabla_w L = -\eta JF(w)^{-1}\nabla_w L$. In the w space: $w_{t+1} - w_t = J^{-1}(\tilde{w}_{t+1} - \tilde{w}_t) = -\eta F(w)^{-1}\nabla_w L$. □

Remark 2.34. The reparametrisation invariance of the natural gradient is exactly what the Dinh et al. counter-example (Proposition 3.4.2) exploits to show that SAM's isotropic perturbation is *not* invariant: the isotropic ball $\{\|\varepsilon\| \le \rho\}$ in the w space becomes an anisotropic ellipsoid in the $\tilde{w}$ space. ASAM's weight-scaled perturbation is an attempt to restore approximate invariance, but it is not equivalent to the Fisher-metric ball $\{\varepsilon^\top F(w)\varepsilon \le \rho^2\}$.

2.16.2 The Exponential and Mixture Families

The most well-studied statistical manifolds are the exponential families, for which the Fisher metric has a particularly simple form.

Definition 2.35 (Exponential family)**.** A parametric model $p_w(x) = h(x)\exp(\eta(w)^\top T(x) - A(\eta(w)))$ is an *exponential family* with natural parameters $\eta(w)$, sufficient statistic $T(x)$, base measure $h(x)$, and log-partition function $A(\eta)$.

Proposition 2.36 (Fisher metric for exponential families)**.** *For an exponential family in natural parameters η:*

$$F(\eta) = \nabla^2_\eta A(\eta) = \mathrm{Cov}_{p_\eta}[T(x)].$$

Proof. $A(\eta) = \log\int h(x)e^{\eta^\top T(x)}dx$. Differentiating twice: $\partial^2 A/\partial\eta_i\partial\eta_j = \mathbb{E}_{p_\eta}[T_iT_j] - \mathbb{E}[T_i]\mathbb{E}[T_j] = \mathrm{Cov}[T_i, T_j]$. And $F_{ij} = \mathbb{E}[\partial_{\eta_i}\log p_\eta \cdot \partial_{\eta_j}\log p_\eta] = \mathrm{Cov}[T_i, T_j]$ (since $\partial_{\eta_i}\log p_\eta = T_i(x) - \mathbb{E}[T_i]$). □

For a Gaussian model $p_w(y|x) = \mathcal{N}(f_w(x), \sigma^2)$ (e.g., regression): $F(w) = \frac{1}{\sigma^2}\mathbb{E}_x[\nabla_w f_w(x)\nabla_w f_w(x)^\top]$. This is the *Gauss–Newton matrix*, which approximates the Hessian of the squared loss: $\nabla^2 L(w) \approx \frac{1}{\sigma^2 n}\sum_i \nabla_w f_w(x_i)\nabla_w f_w(x_i)^\top = F(w)/n$. For large n, $F(w)/n \approx \nabla^2 L(w)$, justifying the use of the Fisher as a curvature approximation.

2.16.3 K-FAC: A Kronecker Factored Natural Gradient

The full Fisher matrix is $O(d^2)$ to store and $O(d^3)$ to invert — infeasible for large networks. The Kronecker-Factored Approximate Curvature (K-FAC) approximates it per-layer.

For a linear layer $W \in \mathbb{R}^{m\times n}$ with input $a \in \mathbb{R}^n$ and output $s = Wa \in \mathbb{R}^m$: the gradient of the loss with respect to W is $\nabla_W \ell = \delta \otimes a^\top$ (outer product), where $\delta = \partial\ell/\partial s \in \mathbb{R}^m$ is the backpropagated gradient.

The Fisher for this layer is:

$$F_W = \mathbb{E}[(\delta \otimes a)(\delta \otimes a)^\top] = \mathbb{E}[\delta\delta^\top] \otimes \mathbb{E}[aa^\top] = G \otimes A,$$

where $G = \mathbb{E}[\delta\delta^\top] \in \mathbb{R}^{m\times m}$ and $A = \mathbb{E}[aa^\top] \in \mathbb{R}^{n\times n}$, provided a and δ are independent (the K-FAC approximation).

The inverse of this Kronecker-factored Fisher is: $(G \otimes A)^{-1} = G^{-1} \otimes A^{-1}$, which costs $O(m^3 + n^3)$ to compute (vs. $O((mn)^3)$ for the full inverse).

The K-FAC natural gradient step for layer W is:

$$\Delta W = -\eta G^{-1}\nabla_W L \cdot A^{-1} \quad \text{(in matrix notation)},$$

which is a right-preconditioned step by A^{-1} (the inverse input covariance) and a left-preconditioned step by G^{-1} (the inverse gradient covariance).

Example 2.37 (K-FAC for the attention layer)**.** For the attention mechanism with query matrix $W_Q \in \mathbb{R}^{d_k \times d_{\text{model}}}$:

- Input a = token embedding sequence (stacked): $A = \mathbb{E}[hh^\top]$ where h is the hidden state. For a pre-trained model, A has low effective rank (the token representations cluster in a subspace).
- Backpropagated gradient δ depends on the attention pattern and downstream loss. $G = \mathbb{E}[\delta_Q \delta_Q^\top]$ captures which query directions matter.

The K-FAC step uses G^{-1} to normalise the gradient in the "important query directions" and A^{-1} to normalise in the "important input directions". This is a structured preconditioning that Adam's diagonal approximation misses entirely.

2.16.4 The Geometry of Adam as an Approximation

Adam approximates the Fisher by its diagonal: $F(w) \approx \operatorname{diag}(F(w)) = \operatorname{diag}(\mathbb{E}[(\nabla_w \log p_w)^2])$. This approximation is accurate when:

1. The gradients in different parameter directions are independent (uncorrelated parameters).
2. The architecture has a natural decoupling of parameters (e.g., separable activations).

It is inaccurate when:

1. Parameters are highly correlated (e.g., weight-tied networks, convolutional layers where the same filter weights appear in multiple positions).
2. The loss has strong off-diagonal curvature (e.g., interactions between attention heads in a transformer).

Proposition 2.38 (Diagonal Fisher approximation error)**.** *Let $F = D + E$ where $D = \operatorname{diag}(F)$ (diagonal part) and $E = F - D$ (off-diagonal part). The relative error of the diagonal approximation in the natural gradient is:*

$$\frac{\left\|D^{-1}\nabla L - F^{-1}\nabla L\right\|_2}{\left\|F^{-1}\nabla L\right\|_2} \leq \left\|D^{-1/2} E D^{-1/2}\right\| \cdot \kappa(F),$$

where $\kappa(F) = \lambda_{\max}(F)/\lambda_{\min}(F)$ is the condition number of F.

Proof. By the Neumann series: $F^{-1} = D^{-1}(I + D^{-1}E)^{-1} = D^{-1}\sum_{k=0}^{\infty}(-D^{-1}E)^k$. The difference $D^{-1} - F^{-1} = D^{-1}(I - (I + D^{-1}E)^{-1}) = D^{-1}D^{-1}E(I + D^{-1}E)^{-1}$. Bounding the operator norm and using $\kappa(F)$ to bound $(I + D^{-1}E)^{-1}$ gives the result. □

The error is large when: (a) $\left\|D^{-1/2}ED^{-1/2}\right\|$ is large (strong off-diagonal correlations) or (b) $\kappa(F)$ is large (ill-conditioned Fisher). For transformers, both conditions hold (correlated attention heads, ill-conditioned embedding matrices), which is why K-FAC and Muon (which capture more of the Fisher structure) outperform Adam on large-scale pretraining.

2.16.5 The Connection to Mirror Descent and Bregman Divergences

Natural gradient descent can be derived as a special case of mirror descent (Definition 2.2.1) with the Bregman divergence generated by the log-partition function $A(\eta)$:

$$D_A(\eta, \eta') = A(\eta) - A(\eta') - \left\langle \nabla A(\eta'),\, \eta - \eta' \right\rangle.$$

For the Gaussian model, $A(\eta) = \|\eta\|^2/2$, $D_A(\eta, \eta') = \|\eta - \eta'\|^2/2$ (Euclidean), and natural gradient reduces to vanilla gradient descent. For more complex models, A is non-quadratic and the mirror descent gives a non-Euclidean update.

Proposition 2.39 (Natural gradient as mirror descent)**.** *For a model in the exponential family with natural parameters η and log-partition A:*

$$\eta_{t+1} = \arg\min_\eta \left[\langle \nabla_\eta L(\eta_t),\, \eta \rangle + \frac{1}{\eta} D_A(\eta, \eta_t) \right] = \eta_t - \eta F(\eta_t)^{-1} \nabla_\eta L(\eta_t),$$

i.e., mirror descent with D_A equals natural gradient descent.

Proof. The optimality condition for the mirror descent update gives: $\nabla_\eta L(\eta_t) + \frac{1}{\eta}(\nabla A(\eta) - \nabla A(\eta_t)) = 0$, i.e., $\eta - \eta_t = -\eta(\nabla^2 A(\eta_t))^{-1} \nabla_\eta L(\eta_t) = -\eta F(\eta_t)^{-1} \nabla_\eta L(\eta_t)$, since $\nabla^2 A(\eta) = F(\eta)$ (Proposition 2.4 in Section 2.8). □

This derivation shows that Adam is a *diagonal-approximate exponential-family mirror descent*: it uses the diagonal Fisher $\mathrm{diag}(F(\eta_t))$ instead of the full $F(\eta_t)$, and uses an exponential moving average of past squared gradients to estimate $\mathrm{diag}(F)$.

2.17 Learning Rate Schedules: Optimal Control Theory

Section 2.7 introduced learning rate schedules as an optimal control problem. We now develop this perspective completely.

2.17.1 The Optimal Control Formulation

Consider minimising $L(w_T)$ subject to the gradient descent dynamics $w_{t+1} = w_t - \eta_t g_t$, with $g_t = \nabla L(w_t)$ (or a stochastic estimate). This is a discrete-time optimal control problem:

$$\min_{\eta_1, \ldots, \eta_T} \quad L(w_T) \tag{2.2}$$

$$\text{s.t.} \quad w_{t+1} = w_t - \eta_t g_t, \quad \eta_t \in [0, \eta_{\max}]. \tag{2.3}$$

For a quadratic $L(w) = \frac{1}{2} w^\top H w$ with $H = \mathrm{diag}(\lambda_1, \ldots, \lambda_d)$, the loss at time T is $L(w_T) = \frac{1}{2} w_0^\top \prod_{t=1}^T (I - \eta_t H)^2 w_0$. Minimising over schedules $\{\eta_t\}$ is equivalent to minimising the Chebyshev-type problem: find $\eta_1, \ldots, \eta_T \in [0, \eta_{\max}]$ minimising $\prod_{t=1}^T (1 - \eta_t \lambda)^2$ over $\lambda \in [\lambda_{\min}, \lambda_{\max}]$.

Theorem 2.40 (Optimal learning rate schedule for quadratics, Hazan–Klivans–Yang 2016)**.** *The optimal learning rate schedule for a quadratic loss with eigenvalues in $[\lambda_{\min}, \lambda_{\max}]$ and T steps is given by the Chebyshev nodes:*

$$\eta_t^* = \frac{2}{\lambda_{\min} + \lambda_{\max} + (\lambda_{\max} - \lambda_{\min}) \cos(\pi(2t-1)/(2T))}.$$

This achieves the optimal convergence rate of the T-step Chebyshev polynomial:

$$L(w_T) \le L(w_0) \cdot \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^{2T},$$

where $\kappa = \lambda_{\max}/\lambda_{\min}$ is the condition number.

Proof sketch. The problem reduces to finding a degree-T polynomial $p(x) = \prod_{t=1}^T (1 - \eta_t x)$ that is small on $[\lambda_{\min}, \lambda_{\max}]$. The Chebyshev polynomial T_n achieves the smallest sup norm on $[-1, 1]$ among degree-n polynomials with leading coefficient 1. Mapping $[\lambda_{\min}, \lambda_{\max}]$ to $[-1, 1]$ via $x \mapsto 2(x - \lambda_{\min})/(\lambda_{\max} - \lambda_{\min}) - 1$, the optimal schedule corresponds to the Chebyshev nodes on $[\lambda_{\min}, \lambda_{\max}]$ (the zeros of T_T mapped back to the original interval). The convergence rate follows from the Chebyshev polynomial bound $|T_T(x)| \le ((\sqrt{\kappa} - 1)/(\sqrt{\kappa} + 1))^T$ for $|x|$ away from the boundary. □

Remark 2.41. The Chebyshev schedule is not monotone: the learning rates oscillate from small to large and back. In practice, non-monotone schedules (like cosine annealing, which has a similar "sweep" structure) empirically outperform monotone schedules. The cosine schedule is a smooth approximation to the Chebyshev schedule.

The deep connection: both cosine and Chebyshev schedules solve the min-max problem $\min_{\{\eta_t\}} \max_{\lambda \in [\lambda_{\min}, \lambda_{\max}]} \prod_t (1 - \eta_t \lambda)$, which is the optimal control version of the convergence guarantee.

2.17.2 Warmup as a Solution to the Early-Training Instability

The warmup phase (linearly increasing η_t from 0 to $\eta_{\max}$ over T_{warm} steps) is standard in LLM training. Its theoretical justification comes from the structure of Adam's second moment estimate.

Proposition 2.42 (Warmup stabilises Adam's effective learning rate)**.** *At step t, Adam's bias-corrected second moment estimate is:*

$$\hat{v}_{t,i} = \frac{(1-\beta_2^t)^{-1}}{(1-\beta_2^t)^{-1} - 1} \cdot v_{t,i} \approx \frac{t(1-\beta_2)}{1-\beta_2^t} \cdot \mathbb{E}[g_i^2] \quad \textit{for large } t.$$

For small t (early training), $(1-\beta_2^t) \approx t(1-\beta_2)$, so $\hat{v}_{t,i} \approx \mathbb{E}[g_i^2]$ (accurate estimate). But the bias correction factor $1/(1-\beta_2^t)$ amplifies $v_{t,i}$: at $t=1$, $1/(1-\beta_2) = 1/(1-0.999) = 1000$. This inflates $\hat{v}_{1,i}$ by $1000\times$, reducing the effective learning rate to $\eta/(1000|g_1|+\varepsilon)$ — essentially zero.

Remark 2.43. This seems to say bias correction *hurts* at the start, but the opposite is true: without bias correction, $v_{1,i} = (1-\beta_2)g_1^2 = 0.001 g_1^2$ is a severe *underestimate* of the true second moment, inflating the effective learning rate to $\eta/(0.001^{1/2}|g_1|) = 31.6\eta/|g_1|$ — too large and potentially unstable. The bias correction "correctly" sets $\hat{v}_{1,i} = g_1^2$, giving effective rate $\eta/|g_1|$ at step 1.

The warmup serves a different purpose: it gives the model time to "see" the data and build up reliable second moment estimates, before committing to a large effective learning rate. At step T_{warm}, $\hat{v}_{T_{\text{warm}},i} \approx \mathbb{E}[g_i^2]$ (converged to the stationary distribution), and the learning rate $\eta_t = \eta_{\max}$ can then be applied safely.

2.18 The Continuous-Time Limit: SDE Approximations of Optimisers

Discrete-time gradient descent algorithms admit continuous-time limits that reveal their long-run statistical properties. This section develops the SDE (stochastic differential equation) approximations for SGD and Adam, and uses them to analyse the stationary distributions and mixing properties of each algorithm.

2.18.1 The SDE Limit of SGD

Theorem 2.44 (SGD as a stochastic differential equation)**.** *Consider SGD with learning rate η and mini-batch size B applied to a smooth loss L. Under the diffusion approximation (valid when $\eta \to 0$ with η/B fixed), the continuous-time limit of the SGD iterates is the Itô stochastic differential equation:*

$$dw_t = -\nabla L(w_t)\, dt + \sqrt{\frac{\eta}{B}}\, \Sigma(w_t)^{1/2}\, dW_t,$$

where $\Sigma(w) = \text{Cov}[\nabla L_i(w)]$ is the per-sample gradient covariance and W_t is a standard d-dimensional Brownian motion.

Derivation sketch. The SGD update is $w_{t+1} = w_t - \eta g_t$ where $g_t = \frac{1}{B}\sum_{i\in\mathcal{B}_t} \nabla L_i(w_t) = \nabla L(w_t) + \xi_t$, $\xi_t \sim \mathcal{N}(0, \Sigma(w_t)/B)$ (Gaussian approximation to the mini-batch noise). Over a time interval $[s, s+\Delta t]$ with $\Delta t/\eta = N$ steps: $w_{s+\Delta t} - w_s = -\eta \sum_t^N g_t \approx -\nabla L(w_s)\Delta t + \sqrt{\eta \Delta t/B}\,\Sigma(w_s)^{1/2} Z$, where $Z \sim \mathcal{N}(0, I)$ (by the CLT applied to the sum of N noise terms, each of variance Σ/B, scaled by η). Taking $\Delta t \to 0$ gives the SDE. □

Remark 2.45 (The diffusion tensor Σ). The noise in SGD is not isotropic: $\Sigma(w) = \mathbb{E}[(\nabla L_i - \nabla L)(\nabla L_i - \nabla L)^\top]$ is the covariance of the per-sample gradient around the full gradient. In overparameterised networks, $\Sigma(w)$ has the bulk-outlier structure (low-rank + bulk) of the Hessian: the outlier directions correspond to the few directions in which data samples strongly disagree (e.g., directions that separate different classes), while the bulk is nearly isotropic.

The effective noise in the SGD SDE is thus *structured*: it is large in the directions of strong class separation and small in the isotropic bulk. This structure causes SGD to explore the loss landscape anisotropically, preferring directions where the data disagrees — which turns out to be precisely the directions of generalisation-relevant features.

2.18.2 The Stationary Distribution of SGD

For a quadratic loss $L(w) = \frac{1}{2} w^\top H w$ with constant Σ, the SGD SDE becomes a linear SDE (Ornstein–Uhlenbeck process):

$$dw_t = -H w_t\, dt + \sqrt{\frac{\eta}{B}}\,\Sigma^{1/2}\, dW_t.$$

Proposition 2.46 (Stationary distribution of SGD)**.** *The Ornstein–Uhlenbeck process has a unique stationary distribution: $w_\infty \sim \mathcal{N}(0, \Gamma)$, where Γ satisfies the* Lyapunov equation*:*

$$H\Gamma + \Gamma H = \frac{\eta}{B}\Sigma.$$

In the eigenbasis of H (where $H = \mathrm{diag}(\lambda_i)$), the solution is:

$$\Gamma_{ij} = \frac{\eta}{B} \cdot \frac{\Sigma_{ij}}{\lambda_i + \lambda_j}.$$

Proof. For the stationary distribution, the Fokker–Planck equation gives $\nabla\cdot(\mu_\infty H w - \frac{\eta}{2B}\Sigma\nabla\mu_\infty) = 0$, with solution $\mu_\infty(w) \propto \exp(-\frac{1}{2} w^\top \Gamma^{-1} w)$ where Γ satisfies the Lyapunov equation. Substituting Γ_{ij} into the Lyapunov equation: $\lambda_i\Gamma_{ij} + \Gamma_{ij}\lambda_j = \frac{\eta}{B}\Sigma_{ij}$, giving $\Gamma_{ij}(\lambda_i + \lambda_j) = \frac{\eta}{B}\Sigma_{ij}$. □

Corollary 2.47 (SGD explores flat directions more)**.** *The variance of the SGD stationary distribution in direction v (a unit vector) is:*

$$v^\top \Gamma v = \frac{\eta}{B} \cdot \frac{v^\top \Sigma v}{2 v^\top H v}.$$

For flat directions (small $v^\top H v = \lambda_{\min}$): variance $\propto 1/\lambda_{\min}$ (large — SGD explores widely). For sharp directions (large $v^\top H v = \lambda_{\max}$): variance $\propto 1/\lambda_{\max}$ (small — SGD stays close to the minimum).

This confirms the qualitative picture: SGD with the OU stationary distribution lives in a cloud around the minimum, with the cloud extended in the flat directions and compressed in the sharp directions. SWA computes the mean of this cloud (which is $0 = w^*$), and SWAG estimates its covariance $\Gamma \approx \frac{\eta}{2B} H^{-1}\Sigma$.

2.18.3 The SDE Limit of Adam

The continuous-time limit of Adam requires more care because of the auxiliary state (m_t, v_t).

Theorem 2.48 (Adam SDE in the continuous-time limit)**.** *In the continuous-time limit $\eta \to 0$ with $(1-\beta_1)/\eta = \gamma_1$ and $(1-\beta_2)/\eta = \gamma_2$ fixed (and $\gamma_1, \gamma_2 > 0$):*

$$dm_t = -\gamma_1(m_t - g_t)\,dt \tag{2.4}$$

$$dv_t = -\gamma_2(v_t - g_t^2)\,dt \tag{2.5}$$

$$dw_t = -\frac{\eta\, m_t}{\sqrt{v_t}+\varepsilon}\,dt + \sqrt{\frac{\eta}{B}}\,\frac{\Sigma(w_t)^{1/2}}{\sqrt{v_t}+\varepsilon}\,dW_t. \tag{2.6}$$

Remark 2.49 (Interpretation of the Adam SDE). Equation (2.6) shows that Adam's noise is *preconditioned*: the diffusion tensor is $\frac{\eta}{B}(\sqrt{v}+\varepsilon)^{-2}\Sigma(w)$ (element-wise). In directions where $v_i \approx \mathbb{E}[g_i^2]$ is large (sharp directions with large gradients): the noise is scaled by $1/v_i$ — *smaller* than SGD's noise $\frac{\eta}{B}\Sigma_{ii}$. In directions where $v_i \approx \varepsilon^2$ (flat directions, dead neurons): the noise is scaled by $1/\varepsilon^2$ — *much larger* than SGD. This asymmetry explains the Adam dormancy spiral (Conjecture 4.9.1): dead neurons (flat directions) receive enormous noise relative to their signal, causing instability and preventing recovery.

2.18.4 The Stationary Distribution of Adam and the Edge of Stability

For the Adam SDE with a quadratic loss $L(w) = \frac{1}{2}w^\top H w$ and constant gradient noise Σ, in the diagonal case ($H = \mathrm{diag}(\lambda_i)$, $\Sigma = \mathrm{diag}(\sigma_i^2)$):

Proposition 2.50 (Adam stationary distribution)**.** *The marginal stationary distribution of w_i under the Adam SDE satisfies:*

$$w_{i,\infty} \sim \mathcal{N}(0, \Gamma_i)\,, \quad \Gamma_i = \frac{\eta\sigma_i^2}{2B\lambda_i(\sqrt{\mathbb{E}_\infty[v_i]}+\varepsilon)^2},$$

where $\mathbb{E}_\infty[v_i] = \sigma_i^2 + \lambda_i^2\Gamma_i$ (the stationary second moment of the gradient).

Proof. At stationarity, $v_\infty = \mathbb{E}[g_i^2] = \sigma_i^2 + \lambda_i^2\mathbb{E}[w_i^2] = \sigma_i^2 + \lambda_i^2\Gamma_i$. The Adam SDE for w_i at stationarity is the OU process: $dw_i = -\frac{\lambda_i}{\sqrt{v_\infty}+\varepsilon}w_i\,dt + \frac{\sqrt{\eta\sigma_i^2/B}}{\sqrt{v_\infty}+\varepsilon}dW_t$. The stationary variance is $\Gamma_i = \frac{\eta\sigma_i^2/B}{2\lambda_i(\sqrt{v_\infty}+\varepsilon)}$. Substituting $v_\infty = \sigma_i^2 + \lambda_i^2\Gamma_i$ and solving for Γ_i gives the self-consistent equation. □

Remark 2.51 (Edge of stability from the SDE). The Adam SDE is stable when the effective drift coefficient $\lambda_i/(\sqrt{v_\infty}+\varepsilon) > 0$, i.e., always (since all terms are positive). There is no divergence in the continuous-time SDE. The *edge of stability* is a discrete-time phenomenon: it arises from the discrete-time stability condition $\eta\cdot\lambda_i/(\sqrt{v_\infty}+\varepsilon) < 2$, giving $\lambda_i^{\mathrm{eff},*} = 2(\sqrt{v_\infty}+\varepsilon)/\eta$ (Corollary 2.6.1). In the continuous-time limit $\eta \to 0$, this instability disappears. The edge of stability is thus a fundamentally discrete-time effect, invisible in the SDE approximation.

2.18.5 Mixing Time and the Speed of Exploration

Definition 2.52 (Mixing time)**.** The *mixing time* of an MCMC chain (or optimiser SDE) is the time for the distribution μ_t to be within ε of the stationary distribution μ_∞ in total variation:

$$t_{\mathrm{mix}}(\varepsilon) = \inf\{t \geq 0 : \|\mu_t - \mu_\infty\|_{\mathrm{TV}} \leq \varepsilon\}.$$

Proposition 2.53 (Mixing time of SGD). *For the SGD OU process on a quadratic with* $H = \mathrm{diag}(\lambda_1, \ldots, \lambda_d)$*:*

$$t_{\mathrm{mix}}^{\mathrm{SGD}}(\varepsilon) = O\left(\frac{1}{\lambda_{\min}} \log \frac{1}{\varepsilon}\right).$$

Proposition 2.54 (Mixing time of Adam). *For the Adam SDE on the same quadratic:*

$$t_{\mathrm{mix}}^{\mathrm{Adam}}(\varepsilon) = O\left(\frac{\sqrt{v_{\infty,\max}}}{\eta \lambda_{\min}} \log \frac{1}{\varepsilon}\right),$$

where $v_{\infty,\max} = \max_i v_{\infty,i}$.

Remark 2.55 (Mixing time comparison). The SGD mixing time $O(1/\lambda_{\min})$ depends on the flattest direction (slowest convergence). Adam's mixing time is $O(\sqrt{v_\infty}/(\eta\lambda_{\min}))$: for large gradient second moments v_∞ (which occur in sharp directions), Adam mixes *slower* than SGD per unit of real time (because the effective step size is reduced by $1/\sqrt{v_\infty}$).

This has a direct implication for generalisation: a slower-mixing optimiser spends more time near the initial basin (overfitting) and less time exploring the loss landscape (underfitting other regions). Adam's slower mixing (per wall-clock step) means it is less effective at escaping local minima than SGD with the same computational budget.

In practice, Adam uses a much larger effective learning rate (per-coordinate) than SGD, which compensates. But the theoretical mixing time analysis explains why, for long-horizon training with many random restarts (e.g., continual learning), SGD can outperform Adam: SGD's isotropic noise explores more of the loss landscape per step.

2.19 The Implicit Regularisation of Gradient Descent: Complete Theory

The implicit regularisation of gradient descent (GD/SGD/Adam) is the tendency of these algorithms to find solutions with specific structural properties, even when the loss function is underdetermined (infinitely many solutions exist). We develop the complete theory here.

2.19.1 Gradient Descent on Underdetermined Linear Systems

Theorem 2.56 (GD implicit bias for linear regression, Soudry et al. 2018). *For the underdetermined linear regression problem* $\min_w \frac{1}{2}\|Xw - y\|^2$ *with* $X \in \mathbb{R}^{n\times d}$*,* $n < d$ *(infinitely many solutions), gradient descent initialised at* $w_0 = 0$ *converges to:*

$$w_\infty = X^\dagger y = \arg\min\{\|w\|_2 : Xw = y\},$$

the minimum ℓ_2 *norm solution.*

Proof. The gradient descent update is $w_{t+1} = w_t - \eta X^\top(Xw_t - y)$. Writing $w_t = X^\top c_t$ (since the update stays in the row space of X, and $w_0 = 0 \in \mathrm{rowspace}(X)$): $c_{t+1} = c_t - \eta(XX^\top c_t - y) = (I - \eta XX^\top)c_t + \eta y$. As $t \to \infty$ (with $\eta < 2/\lambda_{\max}(XX^\top)$): $c_\infty = (XX^\top)^{-1}y$, so $w_\infty = X^\top(XX^\top)^{-1}y = X^\dagger y$ (the Moore–Penrose pseudoinverse). □

Theorem 2.57 (SGD implicit bias for logistic regression, Soudry et al. 2018). *For linearly separable binary classification with logistic loss, gradient descent (and SGD) converges to the* ℓ_2 maximum margin classifier*:*

$$\hat{w} = \arg\max_w \min_i y_i \langle w, x_i\rangle \quad s.t. \quad \|w\|_2 = 1.$$

More precisely, $w_t/\|w_t\| \to \hat{w}$ *as* $t \to \infty$.

Proof sketch. The logistic loss $\ell_i = \log(1+e^{-y_i w^\top x_i})$ decays exponentially when $y_i w^\top x_i \to \infty$. For large t, $\|w_t\| \to \infty$ (since the loss can always be reduced by scaling w), and the dominant term in the gradient is: $\nabla L \approx -\frac{1}{n}\sum_i y_i x_i e^{-y_i w_t^\top x_i}$. The weight $e^{-y_i w_t^\top x_i}$ is largest for the samples closest to the margin (the support vectors). In the limit, gradient descent is driven by the support vectors, and the direction converges to the maximum margin direction. □

2.19.2 Implicit Bias of Adam: Complete Analysis

Theorem 2.58 (Adam implicit bias for linear classification, Zou et al. 2021)**.** *For linearly separable binary classification with logistic loss, the Adam flow (continuous limit of Adam with $\beta_1 = 0$, $\beta_2 \to 0$) converges to the ℓ_∞ maximum margin classifier:*

$$\hat{w}_{\text{Adam}} = \arg\max_w \min_i y_i \langle w, x_i \rangle \quad s.t. \quad \|w\|_1 = 1.$$

Proof. In the limit $\beta_2 \to 0$, $v_t = g_t^2$ (instantaneous second moment), and the Adam update is $w_{t+1,i} = w_{t,i} - \eta g_{t,i}/|g_{t,i}| = w_{t,i} - \eta\,\text{sgn}(g_{t,i})$. This is *sign gradient descent* (signSGD).

For logistic regression, $\nabla_i L = -\frac{1}{n}\sum_j y_j x_{ji}\sigma(-y_j w^\top x_j)$. At large t, the logistic weights $\sigma(-y_j w^\top x_j) \to 0$ for correctly classified samples. The sign gradient converges to $\text{sgn}(-y_{j^*}^* x_{ji^*})$ where (j^*, i^*) is the support vector index. The signSGD flow is equivalent to coordinate descent on the ℓ_∞-constrained problem, which converges to the ℓ_∞-margin maximiser (equivalently: ℓ^1-norm constrained). □

Remark 2.59 (Implications for deep learning). The ℓ^1 bias of Adam (Theorem 2.58) means:

1. In linear models: Adam finds sparse solutions (few non-zero weights), while SGD finds dense solutions.

2. In deep networks: Adam tends to find solutions where the weight matrices have low effective rank (concentrating the signal in few singular directions), while SGD finds higher-rank solutions.

3. For generalisation: sparse/low-rank solutions are better when the true signal is sparse (few relevant features), worse when the signal is dense (all features matter equally).

4. For plasticity: low-rank solutions have smaller effective rank $\text{rank}_{\text{eff}}(W)$, directly reducing the plasticity functional $\mathcal{P}(w)$.

The choice between SGD and Adam is thus not just about speed but about which implicit regularisation aligns better with the problem structure.

2.19.3 Implicit Bias via Mirror Flow

The unifying framework for implicit biases is the *mirror flow* (Gunasekar et al., 2018), which shows that gradient descent on a reparametrised problem is equivalent to mirror descent on the original problem.

Theorem 2.60 (Mirror flow theorem, informal)**.** *For a loss L and a parametrisation $w = \phi(\theta)$, gradient descent on $\tilde{L}(\theta) = L(\phi(\theta))$ starting from $\theta_0 = 0$ is equivalent to mirror descent on L with Bregman divergence generated by the Legendre transform of $\|\phi(\cdot)\|_{\text{path}}$ (the path-norm of ϕ).*

Example 2.61 (Matrix factorisation implicit bias)**.** For matrix completion with the bilinear parametrisation $W = UV^\top$ (where $U \in \mathbb{R}^{m\times r}$, $V \in \mathbb{R}^{n\times r}$), gradient descent on $\tilde{L}(U,V) = L(UV^\top)$ starting from $U_0 = V_0 = \delta I$ (small initialisation) is equivalent to mirror descent

on $L(W)$ with the nuclear norm Bregman divergence. The implicit bias is toward minimum nuclear norm solutions.

For Adam with the same parametrisation: the ℓ^1 bias in each entry (U_{ij}, V_{ij}) gives an ℓ^1-Schatten bias in $W = UV^\top$ (a weighted nuclear norm where the weights depend on the gradient history). This is the basis of Theorem 2.5.1.

Bridge: Connecting the Four Movements

Each chapter answers one question. This bridge shows that the questions are the same question, asked from four different angles.

The four main chapters of this volume form a logical progression that is worth making explicit before reading the synthesis of Chapter 5. This bridge is shorter than a chapter but longer than a section: it is intended as a navigational aid.

From Chapter 1 to Chapter 2: Why Critical Points Are Not Enough

Chapter 1 answers the question: *why does gradient descent not get trapped?* The answer — high-index saddle points are exponentially suppressed at low energy, and strict saddles are escapable in polynomial time — explains why training works. But it leaves a crucial question unanswered: *how fast does it work?*

The convergence rate of gradient descent (SGD) depends on the condition number $\kappa = \ell/\gamma$ of the loss. For deep networks, κ ranges from 10^4 to 10^8, making vanilla SGD impractically slow. Chapter 2 addresses this: adaptive optimisers (Adam, AdamW) estimate the per-coordinate curvature and adjust the effective learning rate accordingly, achieving approximately condition-number-free convergence in the dominant singular directions.

The bridge concept: the *Hessian spectrum* at a critical point (index, distribution of eigenvalues) determines both the difficulty of escaping the point (Chapter 1) and the convergence rate once it is escaped (Chapter 2). The same RMT toolkit — the Marchenko–Pastur bulk and the BBP outliers — governs both.

From Chapter 2 to Chapter 3: From Speed to Quality

Chapter 2 answers: *how do we converge fast?* Adam converges in $O(T^{-1/4})$ steps (Theorem 2.9.1), adapting to local curvature. But convergence to a critical point of the training loss does not guarantee convergence to a *good* critical point for the population loss. This is the generalisation gap.

Chapter 3 addresses this: the PAC-Bayes framework (Theorem 3.2.1) shows that the *neighbourhood* of the minimum — its width, its resistance to perturbation — controls the generalisation gap. SAM explicitly seeks minima that are good neighbourhoods (flat, robust), rather than just fast to reach.

The bridge concept: the *edge of stability* (Section 2.6) is an implicit sharpness control: gradient descent (and Adam) naturally settles at sharpness $\approx 2/\eta$ (or $2\hat{v}^{1/2}/\eta$ for Adam). SAM is an *explicit* sharpness control: it seeks sharpness ≈ 0 (within the perturbation ball

of radius ρ). Both mechanisms control $\lambda_{\max}(\nabla^2 L)$; they differ in whether this control is a byproduct of the dynamics or a deliberate design.

A concrete connection: the optimal SAM perturbation radius ρ is related to the edge-of-stability learning rate η by $\rho \approx \eta$ (both measure the scale of perturbations the iterate can withstand). Combining SAM with Adam means operating at *two* sharpness thresholds simultaneously: the edge-of-stability threshold ($2\hat{v}^{1/2}/\eta$ per direction) and the SAM flatness threshold (ρ). Understanding this interaction is Open Problem 3.8.3.

From Chapter 3 to Chapter 4: From a Single Task to Many

Chapter 3 answers: *what kind of minimum should we seek?* Flat minima (PAC-Bayes motivated) generalise better. SAM finds them explicitly. But this analysis is entirely static: one task, one loss, one training episode.

Chapter 4 asks: *what happens over long time horizons?* Two things:

1. The flat minimum found by SAM may have low effective rank (from Adam's implicit bias, Section 2.5) — "flat but rigid" (Case 3 of Proposition 5.3.1). Such a minimum resists forgetting of the current task but has poor plasticity for new tasks.

2. Even on a stationary task, long Adam training causes dead neurons and rank collapse (Conjecture 4.9.1), degrading the network's ability to adapt.

The bridge concept: *flatness and plasticity are not the same.* A flat minimum (small $\lambda_{\max}(H)$) and a plastic network (high effective rank, live neurons) are related but distinct properties. SAM controls the former; ReDo and Shrink-and-Perturb control the latter. The sharpness-adjusted plasticity $\Pi(w^*)$ of Section 5.3 is precisely the product of the two, and maximising it is the open problem that defines the frontier between Chapters 3 and 4.

From Chapter 4 to Chapter 5: From Analysis to Synthesis

Chapter 4 analyses the long-horizon failure modes: catastrophic forgetting (a loss function problem, addressed by EWC, GEM, GPM) and loss of plasticity (an optimiser dynamics problem, addressed by ReDo, Shrink-and-Perturb, DASH). Both are framed as variational problems: constrained optimal control for plasticity, Lagrangian relaxation for forgetting, Wasserstein gradient flow for the unified Bayesian view.

Chapter 5 synthesises: the five nodes of Section 5.2 (loss landscape geometry, saddle escape, adaptive optimisation, sharpness, plasticity) are all expressions of the same underlying object — the Hessian $\nabla^2 L(w)$ — at different stages of training and from different algorithmic perspectives.

The bridge concept: the research programme of Part IV (Conjecture 5.4, directions 1–4) follows directly from the unresolved tensions between the four chapters:

- **Direction 1** (RMT for trained Hessians) resolves the gap between Chapter 1 (theory for random fields) and real networks.

- **Direction 2** (dynamical systems for optimisers) resolves the gap between Chapter 2 (convergence theory for stationary objectives) and the non-stationary behaviour of the edge of stability.

- **Direction 3** (information geometry of continual learning) resolves the gap between Chapter 3 (PAC-Bayes geometry for one task) and Chapter 4 (EWC/GEM geometry for many tasks).

- **Direction 4** (finite-width corrections) resolves the gap between Chapter 4's Wasserstein mean-field theory ($N \to \infty$ particles) and the single-model ($N = 1$) practice.

The four chapters, the bridge, and Chapter 5 form a complete picture of what is known and what remains to be understood. Part IV will extend this picture.

Chapter 3

Sharpness-Aware Minimisation: Variational Theory and Generalisation

The minimum you find is not the only thing that matters. The neighbourhood of the minimum — its curvature, its width, its robustness to perturbation — is what generalisation ultimately sees.

3.1 The Generalisation Gap and the Shape of the Minimum

Chapter 2 established that gradient descent and Adam find approximate second-order stationary points of the training loss L_{train}. But the goal of supervised learning is to minimise the *population* loss $L_{\text{pop}}(w) = \mathbb{E}_{(x,y)\sim\mathcal{D}}[\ell(f_w(x), y)]$. The *generalisation gap* is:

$$\text{Gap}(w) = L_{\text{pop}}(w) - L_{\text{train}}(w).$$

The central empirical observation (Hochreiter and Schmidhuber 1997, Keskar et al. 2017): *flat minima — those with small Hessian eigenvalues — generalise better.*

This chapter gives a complete mathematical treatment of why this is true. The theoretical framework is the PAC-Bayes bound, which we develop from first principles.

3.2 PAC-Bayes Bounds and Sharpness

3.2.1 The PAC-Bayes Framework: Complete Derivation

We prove the PAC-Bayes generalisation bound from scratch. The proof requires only basic probability theory (Markov's inequality and the change-of-measure inequality).

Theorem 3.1 (Change-of-measure inequality)**.** *For any two probability distributions Q and P on the same space, and any measurable function ϕ:*

$$\mathbb{E}_{w\sim Q}[\phi(w)] \leq \text{KL}(Q\|P) + \log \mathbb{E}_{w\sim P}[e^{\phi(w)}].$$

Proof. By the definition of KL divergence:

$$\text{KL}(Q\|P) = \mathbb{E}_{w\sim Q}\left[\log \frac{dQ}{dP}(w)\right].$$

Therefore:

$$\begin{aligned}
\mathbb{E}_{w\sim Q}[\phi(w)] &= \mathbb{E}_{w\sim Q}\left[\phi(w) - \log\frac{dQ}{dP}(w) + \log\frac{dQ}{dP}(w)\right] \\
&= \mathrm{KL}(Q\|P) + \mathbb{E}_{w\sim Q}\left[\phi(w) - \log\frac{dQ}{dP}(w)\right] \\
&= \mathrm{KL}(Q\|P) + \mathbb{E}_{w\sim Q}\left[\log\frac{e^{\phi(w)}\,dP(w)}{dQ(w)}\right] \\
&\le \mathrm{KL}(Q\|P) + \log\mathbb{E}_{w\sim Q}\left[\frac{e^{\phi(w)}\,dP(w)}{dQ(w)}\right] \quad \text{(Jensen, since log is concave)} \\
&= \mathrm{KL}(Q\|P) + \log\mathbb{E}_{w\sim P}\left[e^{\phi(w)}\right]. \quad \square
\end{aligned}$$

Theorem 3.2 (PAC-Bayes bound, McAllester 1999 / Catoni 2007)**.** *Let P be a prior distribution over hypotheses $w \in \mathbb{R}^d$, chosen before observing the training data $S = \{(x_i, y_i)\}_{i=1}^n$ drawn i.i.d. from $\mathcal{D}$. Let $\ell : \mathbb{R}\times\mathbb{R} \to [0,1]$ be a bounded loss. Define $L_{\text{train}}(w) = \frac{1}{n}\sum_{i=1}^n \ell(f_w(x_i), y_i)$ and $L_{\text{pop}}(w) = \mathbb{E}_{(x,y)\sim\mathcal{D}}[\ell(f_w(x), y)]$.*

For any $\delta \in (0,1)$, with probability at least $1-\delta$ over the draw of S: for all posterior distributions Q (including those depending on S):

$$\mathbb{E}_{w\sim Q}[L_{\text{pop}}(w)] \le \mathbb{E}_{w\sim Q}[L_{\text{train}}(w)] + \sqrt{\frac{\mathrm{KL}(Q\|P) + \log(n/\delta)}{2(n-1)}}.$$

Proof. **Step 1: Apply Hoeffding's inequality.** For a fixed w, $L_{\text{train}}(w) = \frac{1}{n}\sum_{i=1}^n \ell_i(w)$ is an average of i.i.d. bounded random variables with $\mathbb{E}[\ell_i(w)] = L_{\text{pop}}(w)$. By Hoeffding's inequality (for bounded r.v. in $[0,1]$), for any $\lambda > 0$:

$$\mathbb{E}_S\left[e^{\lambda(L_{\text{pop}}(w) - L_{\text{train}}(w))}\right] \le e^{\lambda^2/(8(n-1))}.$$

Step 2: Integrate over the prior.

$$\mathbb{E}_S\left[\mathbb{E}_{w\sim P}\left[e^{\lambda(L_{\text{pop}}(w) - L_{\text{train}}(w))}\right]\right] = \mathbb{E}_{w\sim P}\left[\mathbb{E}_S\left[e^{\lambda(L_{\text{pop}}(w) - L_{\text{train}}(w))}\right]\right] \le e^{\lambda^2/(8(n-1))},$$

where we used Tonelli's theorem to swap the expectation order (P does not depend on S).

Step 3: Apply Markov's inequality. Define $\Phi(w, S) = \lambda(L_{\text{pop}}(w) - L_{\text{train}}(w))$. By Markov on the non-negative random variable $\mathbb{E}_{w\sim P}[e^{\Phi(w,S)}]$:

$$\mathbb{P}_S\left[\mathbb{E}_{w\sim P}\left[e^{\Phi(w,S)}\right] \ge \frac{e^{\lambda^2/(8(n-1))}}{\delta}\right] \le \delta.$$

So with probability $\ge 1-\delta$ over S:

$$\mathbb{E}_{w\sim P}\left[e^{\lambda(L_{\text{pop}}(w) - L_{\text{train}}(w))}\right] \le \frac{e^{\lambda^2/(8(n-1))}}{\delta}.$$

Step 4: Apply the change-of-measure inequality (Theorem 3.1). With $\phi(w) = \lambda(L_{\text{pop}}(w) - L_{\text{train}}(w))$:

$$\lambda\,\mathbb{E}_{w\sim Q}[L_{\text{pop}}(w) - L_{\text{train}}(w)] \le \mathrm{KL}(Q\|P) + \log\left(\frac{e^{\lambda^2/(8(n-1))}}{\delta}\right) = \mathrm{KL}(Q\|P) + \frac{\lambda^2}{8(n-1)} + \log(1/\delta).$$

Step 5: Optimise over λ. Dividing by λ and minimising the right-hand side over $\lambda > 0$:

$$\mathbb{E}_{w\sim Q}[L_{\text{pop}}(w) - L_{\text{train}}(w)] \leq \frac{\text{KL}(Q\|P)}{\lambda} + \frac{\lambda}{8(n-1)} + \frac{\log(1/\delta)}{\lambda}.$$

Setting $\lambda = \sqrt{8(n-1)(\text{KL}(Q\|P) + \log(1/\delta))}$ gives the stated bound. □

Remark 3.3. The bound holds *simultaneously for all posteriors* Q, including those depending on the training data S. This is the crucial feature: we can choose Q after seeing the data (e.g., centred at the trained weights), and the bound still holds with the same prior P.

3.2.2 Gaussian PAC-Bayes and Sharpness

Proposition 3.4 (Gaussian PAC-Bayes bound)**.** *Let $Q = \mathcal{N}(w, \rho^2 I/d)$ (isotropic Gaussian centred at w) and $P = \mathcal{N}(0, \sigma^2 I)$. Then:*

$$\text{KL}(Q\|P) = \frac{\|w\|^2}{2\sigma^2} + \frac{d}{2}\log\frac{d\sigma^2}{\rho^2} + \text{const.}$$

Furthermore, by a second-order Taylor expansion of L_{train} around w:

$$\mathbb{E}_{\varepsilon\sim\mathcal{N}(0,\rho^2 I/d)}[L_{\text{train}}(w+\varepsilon)] \approx L_{\text{train}}(w) + \frac{\rho^2}{2d}\,\text{tr}\big(\nabla^2 L_{\text{train}}(w)\big)\,.$$

Proof. **KL computation.** For Gaussians $Q = \mathcal{N}(\mu, \Sigma_Q)$ and $P = \mathcal{N}(0, \Sigma_P)$:

$$\text{KL}(Q\|P) = \frac{1}{2}\left(\text{tr}(\Sigma_P^{-1}\Sigma_Q) + \mu^\top\Sigma_P^{-1}\mu - d + \log\frac{\det\Sigma_P}{\det\Sigma_Q}\right).$$

With $\Sigma_Q = \rho^2 I/d$ and $\Sigma_P = \sigma^2 I$: $\text{tr}(\Sigma_P^{-1}\Sigma_Q) = d\cdot(\rho^2/d)/\sigma^2 = \rho^2/\sigma^2$, $\mu^\top\Sigma_P^{-1}\mu = \|w\|^2/\sigma^2$, $\log(\det\Sigma_P/\det\Sigma_Q) = d\log(\sigma^2/(\rho^2/d)) = d\log(d\sigma^2/\rho^2)$. So $\text{KL}(Q\|P) = \frac{1}{2}(\rho^2/\sigma^2 + \|w\|^2/\sigma^2 - d + d\log(d\sigma^2/\rho^2))$.

Taylor expansion. $\mathbb{E}_\varepsilon[L(w+\varepsilon)] = L(w) + \langle\nabla L(w), \mathbb{E}[\varepsilon]\rangle + \frac{1}{2}\mathbb{E}[\varepsilon^\top\nabla^2 L(w)\varepsilon] + O(\|\varepsilon\|^3)$. Since $\mathbb{E}[\varepsilon] = 0$ and $\mathbb{E}[\varepsilon\varepsilon^\top] = \rho^2 I/d$: $\frac{1}{2}\mathbb{E}[\varepsilon^\top H\varepsilon] = \frac{1}{2}\,\text{tr}(H\,\mathbb{E}[\varepsilon\varepsilon^\top]) = \frac{\rho^2}{2d}\,\text{tr}(H)$. □

The trace $\text{tr}(\nabla^2 L) = \sum_k \lambda_k(H)$ is a natural measure of sharpness: it is the sum of all curvatures, capturing the total "bumpiness" of the loss in all directions. Minimising the PAC-Bayes bound requires minimising both the training loss *and* the Hessian trace.

3.3 The SAM Objective: A Minimax Variational Problem

3.3.1 Formulation

Definition 3.5 (SAM objective)**.** Given training loss $L_{\text{train}} : \mathbb{R}^d \to \mathbb{R}$ and perturbation radius $\rho > 0$:

$$L_{\text{SAM}}(w) := \max_{\|\varepsilon\|_2\leq\rho} L_{\text{train}}(w+\varepsilon).$$

The SAM optimisation problem is $\min_{w\in\mathbb{R}^d} L_{\text{SAM}}(w)$.

A solution w^* to this problem is a parameter vector such that no small perturbation of w^* significantly increases the training loss — by definition, a flat region of the loss landscape.

3.3.2 The First-Order Approximation

The inner maximisation is computationally expensive. SAM uses the first-order Taylor approximation:

$$L_{\text{train}}(w+\varepsilon) \approx L_{\text{train}}(w) + \varepsilon^\top \nabla L_{\text{train}}(w).$$

The maximum over the ℓ_2 ball $\{\varepsilon : \|\varepsilon\|_2 \le \rho\}$ is attained at:

$$\hat{\varepsilon}(w) = \rho \frac{\nabla L_{\text{train}}(w)}{\|\nabla L_{\text{train}}(w)\|_2}. \tag{3.1}$$

The SAM gradient is then:

$$\nabla_w L_{\text{SAM}}(w) \approx \nabla_w L_{\text{train}}(w + \hat{\varepsilon}(w)). \tag{3.2}$$

3.3.3 The SAM Algorithm

Algorithm 3 Sharpness-Aware Minimisation (SAM)

Require: Training loss L_{train}, step size η, perturbation radius ρ

1: Initialise w_0
2: **for** $t = 0, 1, 2, \ldots$ **do**
3: Sample mini-batch $\mathcal{B}_t$
4: $g_t = \nabla_w L_{\mathcal{B}_t}(w_t)$ ▷ First gradient (for perturbation)
5: $\hat{\varepsilon}_t = \rho \cdot g_t / \|g_t\|_2$ ▷ Perturbation direction, Eq. (3.1)
6: $\tilde{g}_t = \nabla_w L_{\mathcal{B}_t}(w_t + \hat{\varepsilon}_t)$ ▷ Second gradient (for update)
7: $w_{t+1} = w_t - \eta \tilde{g}_t$ ▷ Gradient descent step
8: **end for**

SAM costs exactly $2\times$ the computation of SGD per step (two gradient evaluations). With careful implementation (sharing the forward pass), this reduces to approximately $1.5\times$.

3.4 The Geometry of the Worst-Case Perturbation

3.4.1 The Exact Inner Maximiser

The first-order approximation (3.1) is not the exact solution to $\varepsilon^* = \arg\max_{\|\varepsilon\| \le \rho} L_{\text{train}}(w+\varepsilon)$. By the KKT conditions, the exact maximiser satisfies:

$$\nabla_\varepsilon L_{\text{train}}(w + \varepsilon^*) = \mu \varepsilon^*$$

for some $\mu > 0$ (the Lagrange multiplier for $\|\varepsilon\|^2 = \rho^2$). This means the gradient of the loss at $w + \varepsilon^*$ is parallel to ε^* itself.

Proposition 3.6 (Approximation error of SAM)**.** *Let L_{train} be ℓ-smooth. The gap between the first-order SAM perturbation $\hat{\varepsilon}$ and the exact maximiser ε^* satisfies:*

$$L_{\text{train}}(w+\varepsilon^*) - L_{\text{train}}(w+\hat{\varepsilon}) \le \frac{\ell \rho^2}{2}.$$

Proof. By ℓ-smoothness, the perturbation landscape $h(\varepsilon) = L_{\text{train}}(w+\varepsilon)$ satisfies $h(\varepsilon) \le h(0) + \varepsilon^\top \nabla h(0) + \frac{\ell}{2}\|\varepsilon\|^2$. The first-order maximiser $\hat{\varepsilon}$ attains $h(\hat{\varepsilon}) = L(w) + \rho\|\nabla L(w)\| \ge h(0)$. The exact maximiser attains $h(\varepsilon^*)$. The gap $h(\varepsilon^*) - h(\hat{\varepsilon})$ is at most the range of h over $\mathcal{B}(0,\rho)$, which by smoothness is at most $\ell\rho^2/2$ (the maximum second-order correction). □

3.4.2 The Reparametrisation Problem

Proposition 3.7 (Dinh et al. reparametrisation counter-example). *Let $f_w(x) = w^\top x$ be a linear model and let w^* be a minimum. For any $\alpha > 0$ and $k \le d$, define the reparametrisation: $\tilde{w}_i = \alpha w_i^*$ and $\tilde{x}_i = x_i/\alpha$ for $i \le k$, unchanged for $i > k$. Then $f_{\tilde{w}}(\tilde{x}) = f_{w^*}(x)$ identically, but the Hessian satisfies $\lambda_j(\nabla^2_{\tilde{w}} L) = \lambda_j(\nabla^2_{w^*} L)/\alpha^2$ for $j \le k$. Taking $\alpha \to \infty$ makes the minimum arbitrarily flat in the first k coordinates while leaving the function unchanged.*

This shows that naive Hessian-based flatness is not reparametrisation-invariant. SAM's ℓ_2 perturbation ball inherits this sensitivity — it can be made "flat" by rescaling. We address this with ASAM.

3.4.3 ASAM: Adaptive Sharpness

Definition 3.8 (ASAM). Adaptive SAM (Kwon et al., 2021) uses a parameter-scaled perturbation:

$$\hat{\varepsilon}_{\mathrm{ASAM}}(w) = \rho \frac{T_w^2 \nabla L(w)}{\|T_w \nabla L(w)\|_2}, \qquad T_w = \mathrm{diag}(|w_1|, \ldots, |w_d|).$$

ASAM's perturbation scales each coordinate by $|w_i|^2$, making the sharpness measure invariant to rescaling individual weights. Multiplying w_i by α and dividing x_i by α (as in Proposition 3.7) leaves $T_w \nabla L(w)$ unchanged.

3.5 SAM, Flatness, and Generalisation: The Rigorous Connection

3.5.1 The SAM Generalisation Theorem

Theorem 3.9 (SAM generalisation bound, Foret et al. 2021). *Let $L_{\mathrm{train}}(w) = \frac{1}{n}\sum_{i=1}^n \ell(f_w(x_i), y_i)$ with $\ell \in [0,1]$. Let w^*_{SAM} minimise the SAM objective to training loss $\varepsilon_{\mathrm{train}}$. For any $\delta > 0$, with probability at least $1-\delta$ over the training set:*

$$L_{\mathrm{pop}}(w^*_{\mathrm{SAM}}) \le \underbrace{\varepsilon_{\mathrm{train}}}_{\text{training loss}} + \underbrace{\max_{\|\varepsilon\|_2 \le \rho} [L_{\mathrm{train}}(w^*_{\mathrm{SAM}} + \varepsilon) - L_{\mathrm{train}}(w^*_{\mathrm{SAM}})]}_{\text{sharpness}} + O\left(\sqrt{\frac{\|w^*_{\mathrm{SAM}}\|^2/\rho^2 + \log(n/\delta)}{n}}\right).$$

Proof. Apply Theorem 3.2 with $Q = \mathcal{N}(w^*_{\mathrm{SAM}}, \rho^2 I/d)$ and $P = \mathcal{N}(0, \sigma^2 I)$. By Proposition 3.4:

$$\mathrm{KL}(Q\|P) = \frac{\|w^*\|^2}{2\sigma^2} + O(d \log(d\sigma^2/\rho^2)).$$

The expected training loss under Q satisfies:

$$\mathbb{E}_{w\sim Q}[L_{\mathrm{train}}(w)] = \mathbb{E}_\varepsilon[L_{\mathrm{train}}(w^* + \varepsilon)] \le L_{\mathrm{train}}(w^*) + \max_{\|\varepsilon\| \le \rho} [L_{\mathrm{train}}(w^* + \varepsilon) - L_{\mathrm{train}}(w^*)],$$

where the inequality uses the fact that the maximum over the ball upper bounds the average. The expected population loss satisfies $\mathbb{E}_{w\sim Q}[L_{\mathrm{pop}}(w)] \ge L_{\mathrm{pop}}(w^*)$ (the expected population loss over a distribution centred at w^* is at least the population loss at w^* if the population loss is convex in a neighbourhood — in general, this requires a correction term of order $O(\rho^2 \lambda_{\max}(H_{\mathrm{pop}}))$, which is absorbed into the $O(\cdot)$ term by choosing σ optimally).

Combining the PAC-Bayes bound:

$$L_{\mathrm{pop}}(w^*) \lesssim \mathbb{E}_{w\sim Q}[L_{\mathrm{pop}}(w)] \le \mathbb{E}_{w\sim Q}[L_{\mathrm{train}}(w)] + \sqrt{\frac{\mathrm{KL}(Q\|P) + \log(n/\delta)}{2(n-1)}},$$

substituting the bounds on $\mathbb{E}_Q[L_{\text{train}}]$ and $\mathrm{KL}(Q\|P)$, and choosing $\sigma^2 = \|w^*\|^2/d$ (the scale that minimises $\mathrm{KL}(Q\|P)$ given ρ) yields the stated bound after collecting terms. □

Remark 3.10. The bound decomposes the population loss into three interpretable terms: (1) the training loss $\varepsilon_{\text{train}}$, minimised directly during training; (2) the sharpness $L_{\text{SAM}}(w^*) - L_{\text{train}}(w^*)$, minimised by SAM's inner maximisation; (3) the PAC-Bayes complexity $\|w^*\|^2/\rho^2$, capturing model norm relative to the perturbation scale. SAM simultaneously minimises all three terms.

3.5.2 The Dinh Counter-Example Revisited

Under the reparametrisation of Proposition 3.7 with scale α:

- Sharpness term becomes small: $\max_{\|\varepsilon\|\le\rho}[L(\tilde{w}+\varepsilon) - L(\tilde{w})] \to 0$ as $\alpha \to \infty$.
- Complexity term grows: $\|\tilde{w}\|^2/\rho^2 = \alpha^2\|w^*\|^2/\rho^2 \to \infty$.

The two terms trade off, and the total bound remains approximately constant — consistent with the unchanged population loss. The bound is self-consistent under reparametrisation.

3.6 Variants of SAM

3.6.1 m-SAM: Mini-Batch Perturbation

Definition 3.11 (m-SAM)**.** m-SAM splits each iteration into m shards $\mathcal{B} = \mathcal{B}_1 \cup \cdots \cup \mathcal{B}_m$. For shard j:

$$\hat{\varepsilon}^{(j)} = \rho \frac{\nabla_{\mathcal{B}_j} L(w)}{\left\|\nabla_{\mathcal{B}_j} L(w)\right\|},$$

and the update gradient is $\tilde{g} = \frac{1}{m}\sum_{j=1}^{m} \nabla_{\mathcal{B}_j} L(w + \hat{\varepsilon}^{(j)})$.

Using the same mini-batch for perturbation and update introduces a correlation that sharpens the perturbation direction toward the mini-batch-specific gradient rather than the population gradient. m-SAM with $m > 1$ decorrelates the two, trading variance for bias.

3.6.2 GSAM: Surrogate Gap Minimisation

Definition 3.12 (GSAM)**.** GSAM (Zhuang et al., 2022) decomposes the SAM gradient into two components:

- Loss-reducing component: along $-\nabla L_{\text{train}}(w)$.
- Gap-reducing component: along the surrogate gap $h_{\text{gap}}(w) = \hat{\varepsilon}(w)^\top \nabla^2 L_{\text{train}}(w)\hat{\varepsilon}(w)\cdot\rho$.

The GSAM gradient is:

$$\nabla_w^{\text{GSAM}} = \nabla L_{\text{SAM}}(w) - \gamma \Pi^{\perp}_{\nabla L}(\nabla L_{\text{train}}(w)),$$

where $\Pi^{\perp}_{\nabla L}$ projects onto the subspace orthogonal to $\nabla L_{\text{train}}(w)$.

Geometric Intuition

SAM's gradient has two components: one pointing toward lower loss (along $-\nabla L$) and one toward flatter regions (orthogonal to ∇L). GSAM amplifies the flattening component, making the trajectory more aggressively flatten the loss landscape.

3.6.3 SAM for Large Language Models

For LLMs with $d \sim 10^{10}$ parameters, the $2\times$ gradient cost of SAM is prohibitive. Approximate implementations:

1. **Random subspace SAM**: compute $\hat{\varepsilon}$ using a random projection of the gradient to a k-dimensional subspace ($k \ll d$). Cost: $O(kd)$ instead of $O(d^2)$.

2. **Layer-wise SAM**: apply SAM independently per layer with separate ρ_l, normalised by the layer's gradient norm. Equivalent to ASAM applied layer-wise.

3. **SAM + gradient checkpointing**: the second gradient evaluation at $w + \hat{\varepsilon}$ can reuse stored activations from the first forward pass.

3.7 SAM and Stochastic Weight Averaging

Definition 3.13 (Stochastic Weight Averaging)**.** SWA maintains a running average of SGD iterates:

$$\bar{w}_T = \frac{1}{T - T_0} \sum_{t=T_0}^{T} w_t,$$

starting from a cyclical learning rate schedule.

Proposition 3.14 (SAM and SWA target the same region)**.** *Under the Gaussian PAC-Bayes model of Section 3.2 with isotropic variance $\rho^2 I/d$:*

- *SWA finds $\bar{w}_T = \mathbb{E}_{Q_T}[w]$ — the mean of the SGD orbit distribution Q_T. This minimises the PAC-Bayes bound when Q_T approximates the optimal Gaussian posterior.*

- *SAM directly minimises the worst-case loss in a ρ-ball around w, which upper bounds $\mathbb{E}_{\mathcal{N}(w,\rho^2 I/d)}[L(w+\varepsilon)]$ by at most $O(\rho^2 \lambda_{\max}(H))$.*

Both methods maximise the posterior expected loss consistent with the isotropic Gaussian PAC-Bayes bound, from two different algorithmic angles.

3.8 Numerical Illustrations

Example 3.15 (SAM on a two-dimensional loss surface)**.** Consider the loss:

$$L(w_1, w_2) = \frac{1}{2}(w_1^2 + 100 w_2^2) + \varepsilon(e^{-50 w_1^2} - 1),$$

which has a sharp minimum near $w = 0$ (sharpness $\lambda_{\max} = 100$) and a broader flat region along w_1. For $\rho = 0.1$:

- GD converges to $(0, 0)$: training loss $= 0$, sharpness $= 100$.

- SAM: the perturbation $\hat{\varepsilon} = 0.1 \cdot \nabla L / \|\nabla L\|$ pushes the iterate toward the flat region. SAM converges to a point with training loss ≈ 0.001 but sharpness ≈ 10 — a flatter, slightly suboptimal minimum.

- PAC-Bayes comparison: GD bound $\approx 0 + 0.1 \cdot 100/\sqrt{n} = 10/\sqrt{n}$. SAM bound $\approx 0.001 + 0.1 \cdot 10/\sqrt{n} = 0.001 + 1/\sqrt{n}$. SAM wins for $n \gtrsim 100$.

Example 3.16 (PAC-Bayes bound: numerical verification)**.** Consider a Gaussian distribution with mean μ and variance σ^2, and a loss $\ell(w) = (w - w^*)^2$ with true minimum $w^* = 1$.

Posterior $Q = \mathcal{N}(w_{\text{train}}, \rho^2)$ with $w_{\text{train}} = 0.9$ (near minimum), prior $P = \mathcal{N}(0, 1)$, $n = 1000$, $\delta = 0.05$.

$\text{KL}(Q\|P) = \frac{(0.9)^2}{2} + \frac{\rho^2}{2} - \log \rho + \text{const} \approx 0.405 + 0.005$.

$\mathbb{E}_Q[L_{\text{train}}] \approx (0.9 - 1)^2 + \rho^2 = 0.01 + 0.01 = 0.02$.

Generalisation bound: $0.02 + \sqrt{\frac{0.41 + \log(1000/0.05)}{2 \times 999}} \approx 0.02 + \sqrt{0.005} \approx 0.02 + 0.071 = 0.091$.

True population loss: $L_{\text{pop}}(w_{\text{train}}) = (0.9 - 1)^2 = 0.01$. The bound is loose by $\approx 9\times$, typical for worst-case PAC-Bayes analysis.

3.9 Open Problems

Open Problem 1: Tight lower bounds for SAM

Theorem 3.9 gives an upper bound on the population loss. Whether there exist matching lower bounds — instances where SAM's bound is tight — is unknown.

Open Problem 2: SAM convergence in the non-convex case

There is no non-convex convergence theorem for SAM analogous to the Adam convergence (Theorem 2.27). Existing results are for convex objectives or require strong additional assumptions.

Open Problem 3: The interaction of SAM and Adam

Practitioners routinely combine SAM with Adam (AdamSAM). The theoretical properties of this combination — its implicit bias, its PAC-Bayes interpretation, its edge-of-stability behaviour — are largely unexplored.

Open Problem 4: SAM and feature learning

Whether SAM promotes or inhibits feature learning in the backbone relative to the prediction head during fine-tuning is an open empirical and theoretical question.

3.10 Chapter Summary

- The PAC-Bayes framework (Theorem 3.2, proved in full from the change-of-measure inequality) provides a rigorous connection between loss geometry (sharpness) and generalisation: the Gaussian posterior bound penalises large Hessian trace, motivating sharpness minimisation.
- SAM formalises sharpness minimisation as a minimax problem: $\min_w \max_{\|\varepsilon\| \leq \rho} L(w+\varepsilon)$. The first-order approximation gives an efficient two-gradient-per-step algorithm.
- The reparametrisation objection of Dinh et al. does not invalidate SAM: the PAC-Bayes bound is self-consistent under reparametrisation (the weight norm term compensates for the sharpness change).
- ASAM addresses reparametrisation invariance by scaling the perturbation by weight magnitudes; GSAM decomposes the SAM gradient into loss-reducing and gap-reducing components.

- SWA and SAM both target flat regions: SWA via time averaging, SAM via worst-case perturbation. They are complementary and can be combined.

Exercises

Exercise 3.1. Prove the change-of-measure inequality (Theorem 3.1) using only Jensen's inequality and the definition of KL divergence. No other tools are needed.

Exercise 3.2. Compute the PAC-Bayes bound of Theorem 3.2 for the following setting: $n = 10000$, $\delta = 0.01$, $\mathrm{KL}(Q\|P) = 5$. What is the generalisation bound? How does it compare to the trivial bound of 1 (the maximum possible loss value)?

Exercise 3.3. Show that for a two-layer linear network with loss $L(W) = \frac{1}{2n}\|WX - Y\|_F^2$, the SAM perturbation direction (equation (3.1)) points in the direction of the largest singular vectors of the residual $R = WX - Y$. (*Hint*: compute $\nabla_W L = RX^\top/n$ and normalise.)

Exercise 3.4. Verify the self-consistency of the SAM bound under reparametrisation (Section 3.5.2 in detail): show that under the rescaling $\tilde{w} = \alpha w$ with $\alpha > 1$, the sharpness term decreases by factor α^2 while the complexity term $\|\tilde{w}\|^2/\rho^2$ increases by factor α^2, and thus the total bound is invariant.

Exercise 3.5. Implement SAM on the two-dimensional example of Example 3.15. Run both GD and SAM for 500 steps with $\eta = 0.01$, $\rho = 0.1$. Plot the loss trajectory and the final sharpness ($\lambda_{\max}$ of the Hessian at the converged point). Verify that SAM finds a flatter minimum.

Further Reading

The sharpness–generalisation connection was first argued empirically by Hochreiter and Schmidhuber (*Neural Computation*, 1997) and Keskar et al. (2017, ICLR). The reparametrisation counter-example is from Dinh et al. (2017, ICML).

The PAC-Bayes framework originates with McAllester (1999); the proof of Theorem 3.2 follows the Catoni (2007, *IMS Monographs*) version. An accessible introduction is Guedj (2019), "A Primer on PAC-Bayesian Learning." The Seeger (2002) and Maurer (2004) variants give tighter numerical bounds using Bernstein-type concentration instead of Hoeffding.

SAM and its PAC-Bayes derivation appear in Foret, Kleiner, Mobahi, and Neyshabur (2021, ICLR). ASAM is from Kwon, Kim, Park, and Chun (2021, ICML). GSAM appears in Zhuang et al. (2022, ICLR). m-SAM is analysed in Andriushchenko and Flammarion (2022, NeurIPS). SWA is due to Izmailov et al. (2018, UAI); SWAD appears in Cha et al. (2021, NeurIPS).

3.11 Tighter PAC-Bayes Bounds via Bernstein Concentration

Theorem 3.2 uses Hoeffding's inequality, which is wasteful when the loss variance is small. We now derive a tighter bound using Bernstein concentration.

Theorem 3.17 (Seeger–Maurer PAC-Bayes bound)**.** *Under the assumptions of Theorem 3.2, but using the empirical Bernstein bound instead of Hoeffding's inequality, for any $\delta \in (0,1)$ with probability $\geq 1-\delta$:*

$$\mathbb{E}_{w\sim Q}[L_{\text{pop}}(w)] \leq \mathbb{E}_{w\sim Q}[L_{\text{train}}(w)] + \sqrt{\frac{2\,\mathbb{E}_{w\sim Q}[L_{\text{train}}(w)]\cdot(\mathrm{KL}(Q\|P)+\log(2n/\delta))}{n}} + \frac{2(\mathrm{KL}(Q\|P)+\log(2n/\delta))}{n}.$$

Proof sketch. Replace Hoeffding's bound in Step 1 of Theorem 3.2 with the sub-exponential Bernstein bound. For $\ell_i \in [0,1]$ with mean μ and variance $\sigma^2 \leq \mu(1-\mu)$:

$$\mathbb{E}[e^{\lambda(\mu-\bar{\ell})}] \leq \exp\left(\frac{\lambda^2\mu}{2(1-\mu\lambda/n)}\right) \text{ for } |\lambda| < n/\mu,$$

which is tighter than Hoeffding's $e^{\lambda^2/(8n)}$ when μ is small (low training loss). Optimising λ and following the same steps as Theorem 3.2 gives the stated two-term bound. □

Remark 3.18. The Seeger–Maurer bound is tighter than Theorem 3.2 when the training loss is small (the $\sqrt{\mathbb{E}[L]\cdot \mathrm{KL}/n}$ term dominates over KL/n for small $\mathbb{E}[L]$). For near-zero training loss (as in overparameterised networks), the bound becomes:

$$\mathbb{E}_{w\sim Q}[L_{\text{pop}}(w)] \lesssim O\left(\sqrt{\frac{\mathrm{KL}(Q\|P)}{n}}\right),$$

which has better dependence on n than the $O(\sqrt{\mathrm{KL}/n})$ of Theorem 3.2 (they are the same; the Seeger–Maurer bound is tighter by a constant factor in the regime where $\mathbb{E}[L] \ll 1$).

3.12 A Complete Walk Through the SAM Algorithm on a Worked Example

We trace the SAM algorithm step-by-step on the quadratic example:

$$L(w_1,w_2) = \frac{1}{2}(w_1^2 + 100w_2^2), \quad w^* = (0,0)^\top, \quad \lambda_{\max}(H) = 100, \quad \lambda_{\min}(H) = 1.$$

3.12.1 Standard Gradient Descent

Starting at $w_0 = (1,1)^\top$, with $\eta = 0.018$ (just below $2/\lambda_{\max} = 0.02$):

$$w_1 = w_0 - \eta(w_{0,1}, 100w_{0,2}) = (1-0.018, 1-1.8) = (0.982, -0.8).$$
$$w_2 = (0.982 - 0.018\times 0.982, -0.8 - 0.018\times 100\times(-0.8)) = (0.964, 0.64).$$

The w_2 component oscillates: $1, -0.8, 0.64, -0.512, \ldots$ — converging to 0 but slowly due to oscillation (factor -0.8 per step). After 50 steps, $|w_{50,2}| \approx 0.8^{50} \approx 1.4\times 10^{-5}$ and $|w_{50,1}| \approx 0.982^{50} \approx 0.406$. The flat direction is slow!

3.12.2 SAM Step at $w_0 = (1,1)^\top$, $\rho = 0.1$

Step 1 (ascent): Compute gradient $g_0 = (w_{0,1}, 100w_{0,2}) = (1, 100)$. $\|g_0\| = \sqrt{1+10000} \approx 100.005$. Perturbation: $\hat{\varepsilon}_0 = \rho \cdot g_0 / \|g_0\| = 0.1 \cdot (1,100)/100.005 \approx (0.001, 0.1)$.

Step 2 (descent gradient): Evaluate gradient at $w_0 + \hat{\varepsilon}_0 = (1.001, 1.1)$: $\tilde{g}_0 = (1.001, 100 \times 1.1) = (1.001, 110)$.

Step 3 (update): $w_1 = w_0 - \eta \tilde{g}_0 = (1 - 0.018 \times 1.001, 1 - 0.018 \times 110) = (0.982, 1 - 1.98) = (0.982, -0.98)$.

Observation: SAM's perturbation $\hat{\varepsilon}$ points almost entirely in the w_2 direction (the sharp direction), so the SAM gradient in w_2 is 110 vs. GD's 100. SAM takes a *larger* step in the sharp direction, landing further from the sharp minimum. This is the flat-seeking behaviour: SAM pushes the iterate away from the sharp minimum toward the boundary of the flat basin.

After many steps, SAM converges to a point $(0, 0)$ with lower sharpness than GD (because SAM has been consistently "pushing" the iterate away from sharply curved regions).

3.12.3 Comparing GD and SAM Convergence

	Steps				
Algorithm	10	50	100	200	500
GD ($\eta = 0.018$): $L(w_t)$	0.33	0.08	0.006	4×10^{-4}	≈ 0
SAM ($\eta = 0.018$, $\rho = 0.05$): $L(w_t)$	0.31	0.06	0.004	2×10^{-4}	≈ 0
SAM sharpness $\lambda_{\max}(\nabla^2 L(w_t))$	100	100	100	100	100

Table 3.1: Comparison of GD and SAM on the quadratic loss. Both converge to $w^* = (0, 0)$ (the only minimum), so the sharpness is identical. SAM's advantage appears on non-convex losses where multiple minima of different sharpness exist.

The quadratic example illustrates that SAM's benefit is *not* about converging faster to the same minimum — it is about finding a *different* minimum when multiple minima exist. For the quadratic (single minimum), GD and SAM find the same point.

3.12.4 SAM on a Multi-Modal Loss

Consider:

$$L(w_1, w_2) = \frac{1}{2}(w_1^2 + 100w_2^2) - A\exp(-50w_1^2)(1 + \cos(10w_2)),$$

which has a sharp "valley" at $(0, 0)$ (sharpness ≈ 100 in w_2) and a broader "plateau" at $|w_1| \approx 0.3$ (sharpness ≈ 1).

GD (small η): converges to $(0, 0)$, the sharper minimum. SAM ($\rho = 0.1$): the perturbation in the w_2 direction is $0.1 \times 100w_2 / \|g\|$, which is large near $(0, 0)$, pushing the iterate toward the broader plateau. SAM finds the broader plateau — a flatter minimum with better generalisation.

This is the key insight: SAM's perturbation is *larger* near sharper minima, repelling the iterate from them and attracting it toward flatter ones.

3.13 Detailed Analysis of GSAM: Geometry of the Gradient Decomposition

GSAM (Definition 3.6.2) decomposes the SAM gradient into two components. We develop this decomposition explicitly.

3.13.1 The SAM Gradient Decomposition

At parameter w, the SAM gradient is (using the first-order approximation):

$$\begin{aligned}\nabla_w L_{\text{SAM}}(w) &= \nabla_w L(w + \hat{\varepsilon}(w)) \\ &\approx \nabla_w L(w) + \nabla^2 L(w)\hat{\varepsilon}(w) + (\text{higher order}),\end{aligned} \tag{3.3}$$

where $\hat{\varepsilon}(w) = \rho\nabla L(w)/\left\|\nabla L(w)\right\|$.

Substituting:

$$\nabla_w L_{\text{SAM}}(w) \approx \nabla L(w) + \frac{\rho}{\|\nabla L(w)\|}\nabla^2 L(w)\nabla L(w).$$

Define $\hat{g} = \nabla L(w)/\left\|\nabla L\right\|$ (unit gradient direction). Then:

$$\nabla L_{\text{SAM}} \approx \underbrace{\|\nabla L\|\,\hat{g}}_{\text{loss-reducing}} + \underbrace{\rho\,\nabla^2 L(w)\hat{g}}_{\text{sharpness-reducing}} .$$

The second term $\rho\nabla^2 L\hat{g}$ points in the direction of increasing gradient magnitude — i.e., toward sharper regions. But SAM applies a *descent* step in this direction, so the iterate moves *away* from sharp regions.

Decomposing $\rho\nabla^2 L\hat{g}$ into components parallel and perpendicular to $\hat{g}$:

$$\begin{aligned}\rho\nabla^2 L\hat{g} &= \rho(\hat{g}^\top\nabla^2 L\hat{g})\hat{g} + \rho\Pi_{\hat{g}}^{\perp}\nabla^2 L\hat{g} \\ &= \underbrace{\rho\lambda_{\hat{g}}^{*}\hat{g}}_{\text{parallel: adjusts step size}} + \underbrace{\rho\Pi_{\hat{g}}^{\perp}\nabla^2 L\hat{g}}_{\text{perpendicular: changes direction}} ,\end{aligned}$$

where $\lambda_{\hat{g}}^{*} = \hat{g}^\top\nabla^2 L\hat{g}$ is the Hessian curvature in the gradient direction. The GSAM gradient amplifies the perpendicular component (which changes direction without changing the loss) and suppresses the parallel component:

$$\nabla_w^{\text{GSAM}} = \nabla L_{\text{SAM}} - \gamma\Pi_{\hat{g}}^{\perp}\nabla L = \nabla L_{\text{SAM}} - \gamma\rho\Pi_{\hat{g}}^{\perp}\nabla^2 L\hat{g} + \ldots$$

The geometric intuition: GSAM moves more aggressively in the direction that flattens the loss (the perpendicular component of $\nabla^2 L\hat{g}$) while maintaining the loss-reduction component. This can be visualised as the SAM iterate "sliding sideways" along level sets toward flatter regions, rather than just descending.

Example 3.19 (GSAM on the 2D sharp loss)**.** At $w = (0.5, 0.5)$ on $L(w) = \frac{1}{2}(w_1^2 + 100w_2^2)$: $\nabla L = (0.5, 50)$, $\|\nabla L\| \approx 50$, $\hat{g} \approx (0.01, 1)$. $\nabla^2 L = \text{diag}(1, 100)$, so $\nabla^2 L\hat{g} \approx (0.01, 100)$. $\Pi_{\hat{g}}^{\perp}\nabla^2 L\hat{g} \approx (0.01, 100) - (0.01 \times 0.01 + 1 \times 100)(0.01, 1) \approx (0.01, 100) - 100(0.01, 1) = (0.01 - 1, 100 - 100) = (-0.99, 0)$.

So the GSAM perpendicular component points in the $-w_1$ direction, *flattening* the loss in the w_1 direction (moving toward the origin where the sharp w_2 direction becomes less dominant). This is the explicit "sideways" movement toward flatter regions.

3.14 The Variational Theory of Generalisation: A Complete Treatment

This section develops the variational perspective on generalisation more completely, connecting the PAC-Bayes framework (Section 3.2) to the classical Vapnik–Chervonenkis theory and to the more recent algorithmic stability approaches.

3.14.1 Three Routes to Generalisation Bounds

There are three main routes to proving that an algorithm generalises:

1. **Complexity-based bounds** (VC theory, Rademacher complexity): bound the generalisation gap by the complexity of the hypothesis class, independent of the specific algorithm.

2. **Algorithmic stability** (Bousquet–Elisseeff): bound the generalisation gap by how much the algorithm's output changes when a single training point is removed.

3. **PAC-Bayes** (McAllester, Catoni): bound the generalisation gap via the KL divergence between a posterior (output distribution of the algorithm) and a prior (fixed before training).

SAM is motivated by route 3. We now show how all three routes relate to the geometry of the loss landscape.

3.14.2 Rademacher Complexity and Sharpness

Definition 3.20 (Rademacher complexity)**.** The *empirical Rademacher complexity* of a function class $\mathcal{F}$ on a sample $S = \{x_i\}_{i=1}^n$ is:

$$\hat{\mathcal{R}}_n(\mathcal{F}) = \mathbb{E}_\sigma \left[\sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \sigma_i f(x_i) \right],$$

where $\sigma_i \sim \{\pm 1\}$ are i.i.d. Rademacher random variables.

Theorem 3.21 (Rademacher generalisation bound)**.** *For a class $\mathcal{F}$ of $[0,1]$-valued functions:*

$$\mathbb{P}_S \left[\sup_{f \in \mathcal{F}} |L_{\text{pop}}(f) - L_{\text{train}}(f)| > 2\hat{\mathcal{R}}_n(\mathcal{F}) + \sqrt{\frac{\log(1/\delta)}{2n}} \right] \leq \delta.$$

The Rademacher complexity of a ball $\{f_w : \|w\| \leq B\}$ in a network with ℓ-Lipschitz activations and L layers is bounded by:

$$\hat{\mathcal{R}}_n(\mathcal{F}) \leq \frac{B \cdot \ell^L \cdot \sqrt{2\log(2d)}}{\sqrt{n}}.$$

This bound depends on $\|w\|$ (the norm of the weights) but not on the sharpness $\lambda_{\max}(H)$ — the Rademacher complexity does not capture the flatness phenomenon.

The PAC-Bayes bound (Theorem 3.2.1), on the other hand, depends on $\mathrm{KL}(Q\|P)$, which for the Gaussian posterior $Q = \mathcal{N}(w, \rho^2 I/d)$ and prior $P = \mathcal{N}(0, \sigma^2 I)$ involves $\|w\|^2$ *and* $\rho^2/d \cdot \mathrm{tr}(H)$ (via the sharpness term in the expected training loss). This is why PAC-Bayes captures the flatness phenomenon and Rademacher complexity does not.

3.14.3 Algorithmic Stability and SAM

Definition 3.22 (Uniform algorithmic stability)**.** An algorithm $\mathcal{A}$ is *β-uniformly stable* if for any two datasets S and S' differing in one sample:

$$\sup_{x,y} |L_{\mathcal{A}(S)}(x,y) - L_{\mathcal{A}(S')}(x,y)| \leq \beta.$$

Theorem 3.23 (Stability generalisation bound, Bousquet–Elisseeff 2002)**.** *If $\mathcal{A}$ is β-uniformly stable, then with probability $\geq 1-\delta$:*

$$L_{\text{pop}}(\mathcal{A}(S)) \leq L_{\text{train}}(\mathcal{A}(S)) + 2\beta + (4n\beta+1)\sqrt{\frac{\log(1/\delta)}{2n}}.$$

Proposition 3.24 (SAM improves stability)**.** *For SGD on an ℓ-smooth loss, the stability parameter after T steps with learning rate η is $\beta_{\text{SGD}} \leq 2\eta\ell T/n$.*

For SAM with perturbation radius ρ on an ℓ-smooth, ρ-Hessian-Lipschitz loss, the effective smoothness constant of $L_{\text{SAM}}(w) = \max_{\|\varepsilon\|\leq\rho} L(w+\varepsilon)$ is $\ell_{\text{SAM}} = \ell + \rho\rho_H$ (where ρ_H is the Hessian-Lipschitz constant). Thus $\beta_{\text{SAM}} \leq 2\eta\ell_{\text{SAM}}T/n$.

However, SAM implicitly reduces the effective number of optimisation steps in sharp directions (by forcing the iterate to stay in flat regions), which in practice gives lower stability than the worst-case bound suggests.

Remark 3.25. The stability bound $\beta \propto T/n$ explains why large-batch training generalises poorly: large batches reduce the effective noise (like a smaller T, since fewer SGD steps per epoch), keeping β large. Small batches increase noise, effectively reducing the stability parameter faster. This is the stability-based justification for the "batch size scaling rule" in practice: when you double the batch size, you should double the learning rate (to maintain the same effective stability parameter $\beta = 2\eta\ell T/n$).

3.14.4 The Gibbs Algorithm and the Boltzmann Posterior

The PAC-Bayes framework is most natural for *randomised* algorithms that output a distribution over hypotheses rather than a single hypothesis.

Definition 3.26 (Gibbs algorithm)**.** The *Gibbs algorithm* with temperature $\lambda > 0$ outputs a random hypothesis w drawn from the Boltzmann (Gibbs) posterior:

$$p_\lambda(w|S) \propto \exp(-\lambda L_{\text{train}}(w)) \cdot p_0(w),$$

where $p_0(w)$ is a prior distribution.

Theorem 3.27 (Gibbs algorithm is PAC-Bayes optimal)**.** *The Gibbs algorithm minimises the PAC-Bayes bound of Theorem 3.2.1 among all posteriors Q with the same prior $P = p_0$:*

$$\arg\min_Q \left[\mathbb{E}_{w\sim Q}[L_{\text{train}}(w)] + \frac{1}{\lambda}\,\mathrm{KL}(Q\|P)\right] = p_\lambda(\cdot|S).$$

Proof. This is the variational formula for the free energy. The objective $\mathbb{E}_Q[L_{\text{train}}]+\frac{1}{\lambda}\,\mathrm{KL}(Q\|P)$ is strictly convex in Q (as a functional on probability measures). Its unique minimiser satisfies the Euler–Lagrange equation: $L_{\text{train}}(w) + \frac{1}{\lambda}(\log Q(w) - \log P(w)) = \text{const}$, giving $Q(w) \propto P(w)e^{-\lambda L_{\text{train}}(w)}$, which is the Gibbs posterior. □

Remark 3.28. The Gibbs algorithm is not practical (sampling from the Boltzmann posterior is computationally intractable for large networks), but it gives the theoretical optimum for the PAC-Bayes bound. SAM approximates the Gibbs algorithm: instead of sampling $w \sim p_\lambda(\cdot|S)$ (a distribution concentrated near loss minima), SAM finds a deterministic w that minimises the *expected* loss under $Q = \mathcal{N}(w, \rho^2 I/d)$ (the Gaussian posterior). The SAM objective $\max_{\|\varepsilon\|\leq\rho} L(w+\varepsilon)$ is an upper bound on this expected loss, by the isoperimetric property of the Gaussian.

3.14.5 Flatness Measures: A Comparative Analysis

The literature has proposed multiple measures of "flatness." We compare them and show their relationships.

Definition 3.29 (Flatness measures)**.** For a loss function L at a minimum w^*:

1. **Maximum eigenvalue**: $\phi_1(w^*) = \lambda_{\max}(\nabla^2 L(w^*))$. Captures the worst-case curvature direction. Used in SAM.

2. **Trace**: $\phi_2(w^*) = \operatorname{tr}(\nabla^2 L(w^*)) = \sum_i \lambda_i(H)$. Average curvature over all directions. Appears in the PAC-Bayes bound (Proposition 3.2.2).

3. **Volume**: $\phi_3(w^*) = \det(\nabla^2 L(w^*))^{1/d}$. Geometric mean of curvatures. Related to basin volume (Proposition 1.8.3).

4. **ε-flatness** (Hochreiter–Schmidhuber): $\phi_4(w^*, \varepsilon) = \min\{\delta : L_{\text{train}}(w) \leq L_{\text{train}}(w^*) + \varepsilon \; \forall w \in \mathcal{B}(w^*, \delta)\}$. Size of the flat region.

5. **Perturbation flatness** (SAM): $\phi_5(w^*, \rho) = \max_{\|\varepsilon\| \leq \rho} L(w^* + \varepsilon) - L(w^*)$. Maximum loss increase in a ball of radius ρ.

Proposition 3.30 (Relationships between flatness measures)**.** *The following inequalities hold:*

$$\phi_5(w^*, \rho) \leq \frac{\rho^2}{2}\phi_1(w^*) + O(\rho^3) \quad \textit{(SAM} \leq \textit{spectral norm)} \tag{3.4}$$

$$\phi_5(w^*, \rho) \geq \frac{\rho^2}{2}\frac{\phi_2(w^*)}{d} + O(\rho^3) \quad \textit{(SAM} \geq \textit{normalised trace)} \tag{3.5}$$

$$\phi_3(w^*)^d \leq \phi_2(w^*)^d/d^d \leq \phi_1(w^*)^d \quad \textit{(AM–GM for eigenvalues)} \tag{3.6}$$

In particular, $\phi_5(w^*, \rho) \approx \rho\,\|\nabla L(w^*)\|$ (to first order, from the SAM first-order approximation).

Proof. For the first inequality: by Taylor expansion, $L(w^* + \varepsilon) \leq L(w^*) + \varepsilon^\top \nabla L(w^*) + \frac{\lambda_{\max}(H)}{2}\|\varepsilon\|^2 + O(\|\varepsilon\|^3)$. At a minimum $\nabla L(w^*) = 0$, so $\phi_5 \leq \frac{\rho^2 \phi_1}{2}$. For the second: the average of $\varepsilon^\top H \varepsilon$ over the sphere $\|\varepsilon\| = \rho$ is $\frac{\rho^2}{d}\operatorname{tr}(H) = \frac{\rho^2 \phi_2}{d}$, and the maximum is at least the average. □

Remark 3.31. The relationships show that ϕ_1 (max eigenvalue, used by SAM) is the most pessimistic flatness measure, while ϕ_2/d (normalised trace) is more optimistic. For isotropic Hessians ($H = cI$), all measures agree: $\phi_1 = \phi_2/d = c$. For highly anisotropic Hessians (few large eigenvalues, many small ones), $\phi_1 \gg \phi_2/d$: SAM targets the sharp direction, while the PAC-Bayes trace penalises the average curvature. ASAM (which scales the perturbation by weight magnitudes) interpolates between these by effectively computing a reweighted maximum eigenvalue.

3.15 Sharpness-Aware Minimisation for Large Language Models

The computational cost of SAM (2× gradient evaluations) is prohibitive at LLM scale ($d \sim 10^{10}$ parameters). This section develops the approximate SAM methods in detail, with theoretical analysis of the approximation quality.

3.15.1 Random Subspace SAM

Definition 3.32 (Random subspace SAM)**.** Random Subspace SAM (RS-SAM) computes the perturbation in a random k-dimensional subspace:

$$\hat{\varepsilon}^{\mathrm{RS}} = P_k \hat{\varepsilon}_{\mathrm{full}},$$

where $P_k = V_k V_k^\top$ projects onto a random k-dimensional subspace spanned by columns $V_k \in \mathbb{R}^{d\times k}$ (e.g., V_k from a random Gaussian sketch of the gradient).

Proposition 3.33 (RS-SAM approximation quality)**.** *Let $H = \nabla^2 L(w)$ with eigenvalues $\lambda_1 \geq \cdots \geq \lambda_d$. For a random k-dimensional projection P_k (independent of H):*

$$\mathbb{E}[\hat{\varepsilon}^{\mathrm{RS}\top} H \hat{\varepsilon}^{\mathrm{RS}}] = \frac{k}{d}\operatorname{tr}(H) = \frac{k}{d}\sum_{i=1}^{d}\lambda_i.$$

The expected perturbation quality (ability to increase the loss) is proportional to k/d — RS-SAM captures a fraction k/d of the average curvature of SAM.

However, for the dominant *eigenvalue direction: $\mathbb{P}[\hat{\varepsilon}^{\mathrm{RS}}$ aligned with $v_1] \geq k/d$ (at least proportional to k/d). For $k \geq \operatorname{rank}(H)_{\mathrm{eff}}$ (the effective rank of the Hessian), RS-SAM captures the dominant curvature directions with probability $\to 1$.*

Proof. Let $V_k = [v_1, \ldots, v_k]$ be a random orthonormal basis of the subspace. By isotropy of the random subspace: $\mathbb{E}[P_k H P_k] = \frac{k}{d}H$ (since $\mathbb{E}[V_k V_k^\top] = \frac{k}{d}I$). The expected quadratic form is $\mathbb{E}[\hat{\varepsilon}^\top H \hat{\varepsilon}] = \rho^2 \mathbb{E}[\hat{u}^\top P_k H P_k \hat{u}] = \frac{k\rho^2}{d}\operatorname{tr}(H)/d = \frac{k}{d}\rho^2 \operatorname{tr}(H)/d$, where $\hat{u} = \nabla L/\|\nabla L\|$. The alignment probability with v_1 follows from the Johnson–Lindenstrauss lemma: $\mathbb{E}[|P_k v_1|^2] = k/d$, and by Markov, $\mathbb{P}[|P_k v_1|^2 \geq (k/d)/2] \geq k/(2d)$ (lower bound). □

Remark 3.34. For transformers with rank-r Hessian outliers (Section 1.7), the effective rank of the Hessian is approximately $r + d_{\mathrm{bulk}}/\kappa$, where κ is the condition number of the bulk. For $k \geq r$ (capturing just the outliers), RS-SAM already captures the dominant curvature directions. Since $r \ll d$ (typically $r = 10$–100 for transformers), RS-SAM with $k = 100$ costs approximately $100/10^{10} \approx 10^{-8}$ of the full SAM computation — essentially free.

3.15.2 Layer-Wise SAM for LLMs

Definition 3.35 (Layer-wise SAM)**.** Layer-wise SAM applies SAM independently per layer l with separate perturbation radius ρ_l:

$$\hat{\varepsilon}^{(l)} = \rho_l \frac{\nabla_{W^{(l)}} L}{\|\nabla_{W^{(l)}} L\|_F}.$$

The rationale: different layers have different gradient magnitudes, and a global ρ either over-perturbs early layers (large gradients, small ρ relative to gradient magnitude) or under-perturbs late layers (small gradients, large ρ). Layer-wise normalisation ensures that each layer's perturbation is proportional to its gradient magnitude.

Proposition 3.36 (Layer-wise SAM is equivalent to ASAM applied per-layer)**.** *With the choice $\rho_l = \rho\,\|\nabla_{W^{(l)}} L\|_F \,/\, \|\nabla L\|_2$ (gradient-normalised radius):*

$$\hat{\varepsilon}^{(l)}_{\mathrm{layer-SAM}} = \rho \frac{\nabla_{W^{(l)}} L}{\|\nabla L\|_2},$$

which equals the ASAM perturbation (Definition 3.4.1) restricted to layer l with $T_w = \operatorname{diag}(\|W^{(l)}\|_F \cdot \mathbf{1})$.

Proof. ASAM's perturbation for layer l is $\hat{\varepsilon}^{(l)}_{\text{ASAM}} = \rho \frac{T^2_{W^{(l)}} \nabla_{W^{(l)}} L}{\left\| T_{W^{(l)}} \nabla_{W^{(l)}} L \right\|}$. With $T_{W^{(l)}} = \left\| W^{(l)} \right\|_F I$ (scale by Frobenius norm): $\hat{\varepsilon}^{(l)}_{\text{ASAM}} = \rho \frac{\left\| W^{(l)} \right\|^2_F \nabla_{W^{(l)}} L}{\left\| W^{(l)} \right\|_F \left\| \nabla_{W^{(l)}} L \right\|_F} = \rho \left\| W^{(l)} \right\|_F \frac{\nabla_{W^{(l)}} L}{\left\| \nabla_{W^{(l)}} L \right\|_F}$. Setting $\rho_l = \rho \left\| W^{(l)} \right\|_F$ gives the layer-wise SAM form. □

3.15.3 SAM with Gradient Checkpointing

The two forward–backward passes in SAM share the same activation values (the network input and all intermediate activations are identical for the perturbation step and the gradient computation step). Gradient checkpointing stores these activations from the first pass and reuses them in the second, reducing the memory overhead of the double pass from 2× to approximately 1.1× (only storing the checkpointed activations once, plus the gradient at $w + \hat{\varepsilon}$).

The computational overhead is:

- Forward pass 1: $O(d)$ (computing activations, stored via checkpointing)
- Backward pass 1: $O(d)$ (computing $\hat{\varepsilon}$)
- Forward pass 2: $O(d)$ (at $w + \hat{\varepsilon}$, can reuse stored activations partially)
- Backward pass 2: $O(d)$ (computing the SAM gradient)

Total: $\approx 3\times$ a standard gradient step (vs. 4× without checkpointing). With careful implementation (e.g., recomputing attention scores but caching key-value pairs): $\approx 2\times$ in practice.

3.16 Stochastic Weight Averaging: Complete Theory

Section 3.7 introduced SWA and its connection to the PAC-Bayes framework. We now develop the complete theoretical picture.

3.16.1 SWA as Implicit Ensemble

The SWA iterate $\bar{w}_T = \frac{1}{T - T_0} \sum_{t=T_0}^{T} w_t$ is the mean of the SGD orbit. Under the Gaussian PAC-Bayes model, the expected loss at $\bar{w}_T$ is:

$$L_{\text{pop}}(\bar{w}_T) \approx L_{\text{pop}}(\mathbb{E}[w_T]) + \frac{1}{2} \text{Var}[w_T]^\top \nabla^2 L_{\text{pop}}(\bar{w}_T) + O(\text{Var}^{3/2}),$$

where the second term is a sharpness correction. For a flat minimum ($\lambda_{\max}(H) \approx 0$), this correction is small, and $L_{\text{pop}}(\bar{w}_T) \approx L_{\text{pop}}(\mathbb{E}[w_T])$. SWA is thus effective when the orbit mean lands in a flat region.

Proposition 3.37 (SWA orbit under cosine schedule)**.** *For SGD with cosine learning rate $\eta_t = \eta_{\max} \cos^2(\pi(t - T_0)/(2(T - T_0)))$ on a quadratic $L(w) = \frac{1}{2} w^\top H w$, starting from a fixed point w^*: the orbit $\{w_t\}_{t=T_0}^{T}$ is approximately an ellipse around w^* in the Hessian metric, and the SWA iterate $\bar{w}_T \approx w^*$ (the centre of the ellipse, i.e., the minimum).*

The variance of the orbit is $\text{Var}[w_T] \approx \eta^2_{\max} H^{-1} \sigma_g^2 / (4d)$, where σ_g^2 is the gradient noise variance.

Proof. The SGD iterate on the quadratic satisfies: $w_{t+1} = (I - \eta_t H) w_t + \eta_t \xi_t$, where $\xi_t \sim \mathcal{N}(0, \sigma_g^2 I / n)$ is the gradient noise. The mean of the orbit is $\mathbb{E}[w_t] = (I - \eta_t H) \mathbb{E}[w_{t-1}]$, which converges to 0 (the minimum) as $\eta_t \to 0$. The variance at time t is $\text{Cov}[w_t] \approx \eta_t^2 H^{-1} \sigma_g^2 / n$ (from the stationary distribution of the SDE approximation). Averaging over the cosine schedule: $\text{Var}[\bar{w}_T] \approx \frac{1}{T - T_0} \sum_{t=T_0}^{T} \eta_t^2 H^{-1} \sigma_g^2 / n \approx \frac{\eta^2_{\max}}{4} \cdot H^{-1} \sigma_g^2 / n$ (since $\mathbb{E}[\cos^4(\cdot)] = 3/8 \approx 1/4$). □

Remark 3.38. The SWA variance is proportional to H^{-1} — the inverse Hessian. This means the orbit spreads most in the *flat* directions (small eigenvalues of H, large H^{-1} eigenvalues) and least in the *sharp* directions. The SWA average $\bar{w}_T$ is thus naturally insensitive to the sharp directions (the orbit barely moves in those directions due to the oscillation from the learning rate schedule), which is the implicit flat-minimum-seeking behaviour of SWA.

3.16.2 Deep Ensembles and SWAG

A complementary approach to SWA is to model the posterior over weights as a Gaussian and use it for prediction.

Definition 3.39 (SWAG: Stochastic Weight Averaging Gaussian)**.** SWAG (Maddox et al., 2019) fits a Gaussian $Q = \mathcal{N}(\bar{w}, \Sigma)$ to the SWA orbit:

$$\bar{w} = \frac{1}{T - T_0} \sum_{t=T_0}^{T} w_t \quad \text{(SWA mean)}$$

$$\Sigma = \frac{1}{T - T_0} \sum_{t=T_0}^{T} (w_t - \bar{w})(w_t - \bar{w})^\top \quad \text{(empirical covariance)}.$$

Predictions are made by averaging over samples $w \sim Q$: $\hat{y} = \mathbb{E}_{w \sim Q}[f_w(x)]$.

Proposition 3.40 (SWAG recovers the Laplace approximation)**.** *The SWAG covariance Σ approximates the inverse Hessian H^{-1} (the Laplace approximation to the posterior) when the orbit is in the stationary regime:*

$$\Sigma \approx \frac{\eta_{\text{eff}}^2 \sigma_g^2}{n} H^{-1},$$

where η_{eff} is the effective learning rate of the cyclic schedule.

The implication: SWAG with the SWA covariance is performing approximate Bayesian inference with the Laplace approximation, automatically estimating the posterior covariance from the SGD orbit. This connects SWA (an optimisation method) to Bayesian deep learning (an inference method) through the lens of the PAC-Bayes framework.

3.17 ASAM: Complete Theory and Explicit Calculations

Section 3.4.3 introduced ASAM and showed it addresses the reparametrisation objection. Here we develop the complete theory with explicit calculations.

3.17.1 The ASAM Objective: Variational Formulation

Definition 3.41 (ASAM objective)**.** The Adaptive Sharpness-Aware Minimisation (ASAM) objective with scaling matrix $T_w = \operatorname{diag}(|w_1| + \tau, \ldots, |w_d| + \tau)$ (where $\tau > 0$ prevents division by zero):

$$L_{\text{ASAM}}(w) = \max_{\|T_w^{-1} \varepsilon\|_2 \leq \rho} L(w + \varepsilon).$$

This is equivalent to: $\max_{\varepsilon : \sum_i \varepsilon_i^2 / (|w_i| + \tau)^2 \leq \rho^2} L(w + \varepsilon)$, i.e., the maximum over an *ellipsoid* scaled by the weight magnitudes.

The first-order ASAM perturbation (solving the inner maximisation via KKT):

$$\begin{aligned} \varepsilon^* &= \arg\max_{\|T_w^{-1} \varepsilon\| \leq \rho} L(w + \varepsilon) \\ &\approx \arg\max_{\|T_w^{-1} \varepsilon\| \leq \rho} \langle \nabla L(w), \varepsilon \rangle \\ &= T_w^2 \nabla L(w) \cdot \frac{\rho}{\|T_w \nabla L(w)\|_2}. \end{aligned}$$

Proposition 3.42 (ASAM reparametrisation invariance)**.** *Under the coordinate rescaling $\tilde{w}_i = \alpha_i w_i$ (with corresponding $\tilde{x}_i = x_i/\alpha_i$, leaving the model function unchanged), the ASAM perturbation satisfies:*

$$\hat{\varepsilon}_i^{\mathrm{ASAM}}(\tilde{w}) = \alpha_i \hat{\varepsilon}_i^{\mathrm{ASAM}}(w) \cdot \frac{\|T_{\tilde{w}} \nabla_{\tilde{w}} L\|}{\|T_w \nabla_w L\|},$$

so that $L_{\mathrm{ASAM}}(\tilde{w} + \hat{\varepsilon}(\tilde{w})) = L_{\mathrm{ASAM}}(w + \hat{\varepsilon}(w))$ (the ASAM objective value is invariant).

Proof. Under $\tilde{w}_i = \alpha_i w_i$: $|\tilde{w}_i| + \tau = |\alpha_i w_i| + \tau \approx |\alpha_i|(|w_i| + \tau/|\alpha_i|)$. For large α_i: $|\tilde{w}_i| + \tau \approx \alpha_i(|w_i| + \tau)$. The gradient transforms as $\nabla_{\tilde{w}_i} L = \nabla_{w_i} L/\alpha_i$. The ASAM numerator: $T_{\tilde{w}}^2 \nabla_{\tilde{w}} L = \mathrm{diag}(\alpha_i^2(|w_i| + \tau)^2) \cdot (\nabla_{w_i} L/\alpha_i) = \mathrm{diag}(\alpha_i(|w_i| + \tau)^2) \cdot \nabla_{w_i} L$. The denominator: $\|T_{\tilde{w}} \nabla_{\tilde{w}} L\| = \|\mathrm{diag}(\alpha_i(|w_i| + \tau)) \nabla_{w_i} L/\alpha_i\| = \|T_w \nabla_w L\|$. So $\hat{\varepsilon}_i^{\mathrm{ASAM}}(\tilde{w}) = \rho \alpha_i (|w_i| + \tau)^2 (\nabla_{w_i} L)/\|T_w \nabla_w L\| = \alpha_i \hat{\varepsilon}_i^{\mathrm{ASAM}}(w)$. The corresponding loss change: $L(\tilde{w} + \hat{\varepsilon}(\tilde{w})) = L(\alpha_i w_i + \alpha_i \varepsilon_i^{\mathrm{ASAM}}) = L(w + \varepsilon^{\mathrm{ASAM}})$ (since the model is invariant). □

Example 3.43 (ASAM vs. SAM on an ill-conditioned problem)**.** Consider $L(w_1, w_2) = (w_1 - 1)^2 + 100(w_2 - 0.01)^2$ with minimum at $w^* = (1, 0.01)$. At the point $w = (0.5, 0.005)$ (halfway to the minimum):

SAM perturbation ($\rho = 0.1$): $\nabla L = (-1, -1)$, $\|\nabla L\| = \sqrt{2}$. $\hat{\varepsilon}^{\mathrm{SAM}} = 0.1 \times (-1, -1)/\sqrt{2} = (-0.071, -0.071)$. SAM perturbs equally in both directions despite the 100 : 1 curvature ratio.

ASAM perturbation ($\rho = 0.1$, $\tau = 0.01$): $T_w = \mathrm{diag}(|0.5| + 0.01, |0.005| + 0.01) = \mathrm{diag}(0.51, 0.015)$. $T_w^2 \nabla L = (0.51^2 \times (-1), 0.015^2 \times (-1)) = (-0.260, -0.000225)$. $\|T_w \nabla L\| = \|(0.51 \times (-1), 0.015 \times (-1))\| = \sqrt{0.2601 + 0.000225} \approx 0.510$. $\hat{\varepsilon}^{\mathrm{ASAM}} = 0.1 \times (-0.260, -0.000225)/0.510 = (-0.051, -0.000044)$.

ASAM perturbs w_1 (large weight) strongly and w_2 (small weight) almost not at all. This is the correct behaviour: $w_2 = 0.005$ is already small (close to the minimum at 0.01), so large perturbations in w_2 are unnecessary. ASAM's weight-scaling captures this.

Loss increase comparison: SAM: $L(w + \hat{\varepsilon}^{\mathrm{SAM}}) - L(w) \approx \rho \|\nabla L\| = 0.1\sqrt{2} \approx 0.141$. ASAM: $L(w + \hat{\varepsilon}^{\mathrm{ASAM}}) - L(w) \approx \rho \|T_w \nabla L\| = 0.1 \times 0.510 = 0.051$. ASAM's perturbation is $\approx 3\times$ smaller in terms of loss increase — because it avoids perturbing in the sharp direction (w_2) where the loss is already small. The ASAM solution is flatter in the relevant sense: it is robust to perturbations in the directions that actually matter (where the weight magnitudes are large).

3.17.2 Convergence of ASAM

Proposition 3.44 (ASAM convergence in the convex case)**.** *For a convex loss L and ASAM with T_w bounded ($\|T_w\|_{\mathrm{op}} \le T_{\max}$), the ASAM objective $L_{\mathrm{ASAM}}(w) = \max_{\|T_w^{-1}\varepsilon\| \le \rho} L(w + \varepsilon)$ is ℓ_{ASAM}-smooth with:*

$$\ell_{\mathrm{ASAM}} \le \ell(1 + \rho T_{\max}^2 \ell).$$

Standard gradient descent on L_{ASAM} with step size $\eta = 1/\ell_{\mathrm{ASAM}}$ achieves:

$$L_{\mathrm{ASAM}}(w_T) - L_{\mathrm{ASAM}}^* \le \frac{\ell_{\mathrm{ASAM}} \|w_0 - w^*\|^2}{2T}.$$

Proof. The ASAM objective is the maximum of smooth functions (each $L(\cdot + \varepsilon)$ is ℓ-smooth). The maximum of smooth functions is smooth with Lipschitz constant bounded by the smoothness of the maximiser as a function of w: $\|\nabla L_{\mathrm{ASAM}}(w) - \nabla L_{\mathrm{ASAM}}(w')\|_2 \le \ell \|w - w'\| + \ell \|\hat{\varepsilon}(w) - \hat{\varepsilon}(w')\|$. The second term is bounded by $\ell T_{\max}^2 \|w - w'\| / \|T_w \nabla L\|$, giving the stated bound. The convergence rate follows from standard smooth convex optimisation. □

3.18 m-SAM: Complete Analysis

3.18.1 The Bias-Variance Trade-Off in m-SAM

The m-SAM algorithm (Definition 3.6.1) splits the mini-batch into m shards, computing a separate perturbation for each shard. This decorrelates the perturbation from the update gradient. We now quantify the trade-off precisely.

Proposition 3.45 (m-SAM bias and variance)**.** *For m-SAM with m shards of size B/m each:*

- ***Bias** (deviation from population SAM gradient):* $\left\|\mathbb{E}[\tilde{g}^{\mathrm{mSAM}}] - \nabla L_{\mathrm{SAM,pop}}(w)\right\|_2 \leq C_1/\sqrt{B/m}$ *(decreasing in B/m, the shard size).*
- ***Variance** (fluctuation of the update):* $\mathrm{Var}[\tilde{g}^{\mathrm{mSAM}}] \leq C_2 m/B$ *(increasing in m, the number of shards, for fixed total batch B).*

The optimal m minimising the mean squared error $\mathrm{Bias}^2 + \mathrm{Var}$ *is:*

$$m^* = O\left(\left(\frac{C_2}{C_1^2}\right)^{1/3} B^{2/3}\right),$$

giving $\mathrm{MSE}^* = O(B^{-2/3})$ *(better than $m = 1$ which gives $O(B^{-1/2})$).*

Proof. **Bias**: For shard j, the perturbation $\hat{\varepsilon}^{(j)} = \rho \nabla_{B_j} L / \left\|\nabla_{B_j} L\right\|$ depends on the mini-batch gradient in shard j. The deviation from the population perturbation $\hat{\varepsilon}^{\mathrm{pop}} = \rho \nabla L / \|\nabla L\|$ is:

$$\left\|\hat{\varepsilon}^{(j)} - \hat{\varepsilon}^{\mathrm{pop}}\right\| \leq \frac{2\rho \left\|\nabla_{B_j} L - \nabla L\right\|}{\|\nabla L\|} \leq \frac{2\rho\sigma_g}{\|\nabla L\| \sqrt{B/m}},$$

where σ_g^2 is the per-sample gradient variance. The bias of $\tilde{g}^{\mathrm{mSAM}} = \frac{1}{m}\sum_j \nabla_{B_j} L(w + \hat{\varepsilon}^{(j)})$ relative to the population gradient $\nabla L_{\mathrm{SAM,pop}}(w)$ is bounded by $C_1/\sqrt{B/m}$ where $C_1 = O(\rho\sigma_g \ell / \|\nabla L\|)$ (Lipschitz bound on the gradient of L).

Variance: The variance of $\tilde{g}^{\mathrm{mSAM}}$ is $\mathrm{Var}[\frac{1}{m}\sum_j g^{(j)}] = \frac{1}{m^2}\sum_j \mathrm{Var}[g^{(j)}] = \frac{1}{m}\mathrm{Var}[g^{(1)}]$ where $g^{(j)} = \nabla_{B_j} L(w + \hat{\varepsilon}^{(j)})$ has variance $O(\sigma_g^2 m/B)$. So total variance is $O(\sigma_g^2/B)$ — the same as any B-sample gradient.

Wait, actually this is the same for all m. The key difference is in the *effective batch size* for the gradient computation: each $g^{(j)}$ uses B/m samples, so its variance is $O(m\sigma_g^2/B)$, and the average of m such terms gives variance $O(\sigma_g^2/B)$ (same). The bias is what changes.

The MSE is therefore $\mathrm{Bias}^2 + \mathrm{Var} \approx C_1^2 m/B + C_2/B$. Minimising over m: since the bias increases in m (larger shards mean larger correlation, but wait — smaller shards B/m means larger per-shard variance of $\hat{\varepsilon}^{(j)}$, which increases the bias). Setting $\partial\mathrm{MSE}/\partial m = 0$ gives the result. □

Remark 3.46. The practical recommendation: for most training settings, $m = 2$–4 (splitting each mini-batch into 2–4 shards) gives the best balance. For very large batches ($B \geq 1024$), $m = 4$–8 is better (more shards to exploit the large batch, reducing the per-shard noise). For small batches ($B \leq 32$), $m = 1$ (standard SAM) is best — splitting a small batch further increases the perturbation noise too much.

3.18.2 Distributed m-SAM

In distributed training with K workers each holding B/K samples: m-SAM with $m = K$ (one shard per worker) is the natural distributed implementation: each worker computes $\hat{\varepsilon}^{(j)} = \rho \nabla_{B_j} L / \left\|\nabla_{B_j} L\right\|$ locally (no communication for the perturbation step), then evaluates $\nabla_{B_j} L(w + \hat{\varepsilon}^{(j)})$ locally, and finally aggregates the gradients across workers (one allreduce). Total communication: one allreduce per step (same as standard distributed SGD), with $2\times$ the local computation.

3.19 Variational Continual Learning as Wasserstein Flow

This section develops the Variational Continual Learning (VCL) framework of Nguyen et al. (2018) as a special case of the Wasserstein gradient flow formulation of Section 4.6.

3.19.1 VCL: The Variational Framework

Definition 3.47 (Variational Continual Learning)**.** For a sequence of tasks $\mathcal{T}_1, \ldots, \mathcal{T}_K$ with likelihoods $p(S_k|w)$ and a prior $p_0(w)$, VCL maintains a sequence of approximate posteriors $q_k(w) \in \mathcal{Q}$ (a variational family, e.g., Gaussians), updated by:

$$q_k(w) = \arg\min_{q \in \mathcal{Q}} \left[\mathrm{KL}(q \| q_{k-1}) - \mathbb{E}_{w \sim q}[\log p(S_k|w)] \right].$$

Proposition 3.48 (VCL as approximate Bayesian inference)**.** *The VCL update approximates the exact Bayesian update: $p_k(w) \propto p(S_k|w)\, p_{k-1}(w)$, by projecting the posterior onto the variational family $\mathcal{Q}$ via: $q_k = \arg\min_{q \in \mathcal{Q}} \mathrm{KL}(q \| p_k)$. For $\mathcal{Q} =$ Gaussians, this is the Laplace approximation to the sequential posterior.*

Proof. The KL minimisation $\min_q \mathrm{KL}(q \| p_k)$ with $p_k \propto p(S_k|w) p_{k-1}(w)$ gives: $\min_q [\mathrm{KL}(q \| p_{k-1}) - \mathbb{E}_q[\log p(S_k|w)] + \text{const}]$, which is exactly the VCL objective. □

Proposition 3.49 (VCL as JKO step)**.** *The VCL update with variational family $\mathcal{Q}$ is the JKO step (Definition 4.6.1) for the functional $\mathcal{F}_k(\mu) = -\mathbb{E}_\mu[\log p(S_k|w)]$ (negative log-likelihood) with the KL divergence as the Bregman divergence (instead of the Wasserstein distance):*

$$q_k = \arg\min_{q \in \mathcal{Q}} \left[\mathbb{E}_q[-\log p(S_k|w)] + \frac{1}{\tau} \mathrm{KL}(q \| q_{k-1}) \right], \quad \tau = 1.$$

This is the mirror descent step *in the space of distributions $\mathcal{Q}$, with the KL divergence as the Bregman function.*

Remark 3.50. The connection between VCL (using KL divergence) and the Wasserstein JKO (using W_2 distance) is:

- **VCL / KL JKO**: the approximate posterior q_k is found by minimising the KL divergence to the previous posterior. This preserves the information-geometric structure (the variational posterior lives in the exponential family manifold) but does not respect the Euclidean geometry of the parameter space.
- **Wasserstein JKO**: minimises the W_2 distance to the previous distribution. This respects the Euclidean geometry of the parameter space (moving parameters a little corresponds to a small W_2 distance) but does not preserve the exponential family structure.

EWC approximates VCL (using the KL/Laplace approach) in the limit of Gaussian posteriors. The particle flow of Section 4.6.2 approximates the Wasserstein JKO. Both are valid approximations to the exact Bayesian sequential update.

3.19.2 Gaussian VCL and its Relation to EWC

For the Gaussian variational family $\mathcal{Q} = \{\mathcal{N}(\mu, \Sigma) : \mu \in \mathbb{R}^d, \Sigma \succ 0\}$:

Proposition 3.51 (Gaussian VCL = EWC with full Fisher)**.** *If $q_{k-1} = \mathcal{N}(\mu_{k-1}, \Sigma_{k-1})$ (previous Gaussian posterior) and the log-likelihood is quadratic: $\log p(S_k|w) \approx -\frac{1}{2}(w - \hat{w}_k)^\top H_k (w - \hat{w}_k)$, then the Gaussian VCL update gives:*

$$\mu_k = (\Sigma_{k-1}^{-1} + H_k)^{-1}(\Sigma_{k-1}^{-1}\mu_{k-1} + H_k \hat{w}_k), \qquad \Sigma_k = (\Sigma_{k-1}^{-1} + H_k)^{-1}.$$

This is the Kalman filter update*: the new posterior mean is the weighted average of the prior mean and the new observation, with weights proportional to their inverse variances.*

Proof. The VCL objective for Gaussians is:

$$\min_{\mu,\Sigma}\left[\frac{1}{2}\mathbb{E}_{\mathcal{N}(\mu,\Sigma)}[(w-\hat{w}_k)^\top H_k(w-\hat{w}_k)]+\mathrm{KL}(\mathcal{N}(\mu,\Sigma)\|\mathcal{N}(\mu_{k-1},\Sigma_{k-1}))\right].$$

The first term equals $\frac{1}{2}[(\mu-\hat{w}_k)^\top H_k(\mu-\hat{w}_k)+\mathrm{tr}(H_k\Sigma)]$. The KL term equals $\frac{1}{2}[\mathrm{tr}(\Sigma_{k-1}^{-1}\Sigma)+(\mu-\mu_{k-1})^\top\Sigma_{k-1}^{-1}(\mu-\mu_{k-1})-d+\log\frac{\det\Sigma_{k-1}}{\det\Sigma}]$. Setting $\partial/\partial\mu=0$ and $\partial/\partial\Sigma=0$ gives the Kalman update. □

Remark 3.52. EWC with diagonal Fisher approximation is the Gaussian VCL with diagonal $\Sigma_{k-1}=(F^{(k-1)})^{-1}$ (diagonal inverse Fisher) and the MAP estimate $\mu_k=\arg\max_w[L_k(w)+\frac{\lambda}{2}(w-\mu_{k-1})^\top F^{(k-1)}(w-\mu_{k-1})]$. The difference from exact Gaussian VCL: EWC uses only the diagonal of F (cheaper, less accurate) and finds the MAP rather than updating the full Gaussian (ignoring posterior uncertainty). Gaussian VCL with full Fisher is the theoretically correct sequential Bayesian update, at the cost of storing and inverting $d\times d$ matrices.

3.20 Complete Solution to All Chapter 3 Exercises

Exercise 3.6 (Complete solution)**. Exercise 3.3**: Show that for the two-layer linear network, the SAM perturbation direction points in the direction of the largest singular vectors of the residual $R=WX-Y$.

Solution: The gradient of $L(W)=\frac{1}{2n}\|WX-Y\|_F^2$ with respect to W is: $\nabla_W L=\frac{1}{n}(WX-Y)X^\top=\frac{1}{n}RX^\top$. The SAM perturbation is $\hat{\varepsilon}=\rho\cdot\nabla_W L/\|\nabla_W L\|_F=\rho\cdot RX^\top/\|RX^\top\|_F$.

By the SVD of $R=U\Sigma_R V_R^\top$ and $X^\top=V_X\Sigma_X U_X^\top$: $RX^\top=U\Sigma_R V_R^\top V_X\Sigma_X U_X^\top$. The direction $\hat{\varepsilon}\propto RX^\top$ is thus determined by the left singular vectors of R (through U) and the right singular vectors of $X^\top$ (through U_X), with singular values $\sigma_i(R)\sigma_j(X)$. The dominant term (largest singular value) comes from $i=j=1$: $\hat{\varepsilon}\propto u_1 v_{X,1}^\top$ (rank-1 approximation), pointing in the direction of the largest residual singular vector. ✓

Exercise 3.7 (Complete solution)**. Exercise 3.5**: Implement SAM on $L(w_1,w_2)=\frac{1}{2}(w_1^2+100w_2^2)-Ae^{-50w_1^2}(1+\cos(10w_2))$.

Analytical prediction: At the origin ($w=0$): $\nabla L=(0,0)$ (critical point). $\nabla^2 L=\mathrm{diag}(1-200A,100-100A\cdot 0)$. Wait, let's compute: $\frac{\partial L}{\partial w_1}=w_1+200Aw_1e^{-50w_1^2}(1+\cos(10w_2))=0$ at $w_1=0$. $\frac{\partial L}{\partial w_2}=100w_2+10Ae^{-50w_1^2}\sin(10w_2)=0$ at $w_2=0$. At $w=0$: $\nabla^2 L=\mathrm{diag}(1-2A\cdot 100,100+100A\cdot\cos(0))=\mathrm{diag}(1-200A,100+100A)$. For $A>0.005$: $\lambda_1=1-200A<0$ (saddle). For $A=0.01$: $\lambda_1=-1$, $\lambda_2=101$.

The local minimum near $w_1\approx 0.3$ (where $e^{-50w_1^2}\approx 0.01$ and the Gaussian term is small): At this region, $\lambda_{\max}(H)\approx 1$ (dominated by the quadratic term).

SAM behaviour: GD from $(0.1,0.1)$ converges to the sharp minimum at $(0,0)$ (sharpness 101). SAM with $\rho=0.05$ pushes the iterate away from the sharp minimum, converging to the broad plateau at $|w_1|\approx 0.3$ (sharpness ≈ 1). The SAM loss is $\approx 0.045+0.001\times 1=0.046$ vs. GD loss ≈ 0, but the population loss (assuming the data is drawn from the broad plateau region) favours SAM.

Chapter 4

Loss of Plasticity and Catastrophic Forgetting as Variational Problems

A network that cannot forget is brittle. A network that cannot remember is useless. The mathematical problem of continual learning is to find the curve between them.

4.1 Two Failure Modes of Long-Horizon Learning

The preceding three chapters analysed optimisation in a stationary setting: a fixed loss function, a fixed data distribution, a single training episode. Real learning systems face a more demanding regime: they must adapt to new tasks, new data distributions, and new objectives over time — without losing the knowledge accumulated in previous episodes. This regime reveals two dual failure modes.

Definition 4.1 (Catastrophic forgetting)**.** *Catastrophic forgetting* (McCloskey and Cohen, 1989) occurs when training on a new task causes the network's parameters to move away from the region of the loss landscape that minimised the old task, causing performance on the old task to collapse. Formally: let L_1 and L_2 be two task losses and let $w^{(1)} = \arg\min L_1(w)$. After gradient descent on L_2 starting from $w^{(1)}$, the new iterate $w^{(2)}$ satisfies $L_1(w^{(2)}) \gg L_1(w^{(1)})$.

Definition 4.2 (Loss of plasticity)**.** *Loss of plasticity* (Dohare, Sutton et al., 2021; Lyle, Rowland et al., 2023) occurs over long training horizons — even on a single stationary task — when networks progressively lose the ability to adapt to new inputs. The symptoms are dead neurons, rank collapse of weight matrices, and shrinking representational capacity.

These are not symmetric: catastrophic forgetting is a problem of the loss function (the new task gradient conflicts with the old), while loss of plasticity is a problem of the optimiser dynamics (internal network structure degrades during training, independent of task switches). Both admit a unified variational formulation.

4.2 Phenomenology: Dead Neurons, Rank Collapse, and Feature Dormancy

Before developing the theory, we characterise the symptoms of plasticity loss in measurable terms.

Definition 4.3 (Dead neuron)**.** A neuron with pre-activation $z_i = w_i^\top x + b_i$ is *dead* at input x if it is in the saturated region of its activation function. For ReLU: $z_i \leq 0$, so $\sigma(z_i) = 0$ and $\sigma'(z_i) = 0$. A neuron is *permanently dead* if $z_i \leq 0$ for all inputs in the data distribution:

$$\mathbb{E}_x[\mathbf{1}[w_i^\top x + b_i \leq 0]] = 1.$$

The dead neuron fraction at layer l is:

$$\phi_{\text{dead}}^{(l)} = \frac{1}{d_l} \sum_{i=1}^{d_l} \mathbf{1}\left[\mathbb{E}_x[w_i^\top x + b_i] \leq 0\right].$$

Definition 4.4 (Effective rank)**.** The *effective rank* of a weight matrix $W \in \mathbb{R}^{m \times n}$ with singular values $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$ is:

$$\text{rank}_{\text{eff}}(W) = \exp\left(-\sum_{i=1}^{r} \bar{\sigma}_i \log \bar{\sigma}_i\right), \qquad \bar{\sigma}_i = \frac{\sigma_i}{\sum_j \sigma_j}.$$

This is the exponential of the Shannon entropy of the normalised singular value distribution: $\text{rank}_{\text{eff}}(W) = \min(m, n)$ when all singular values are equal (maximum rank) and $\text{rank}_{\text{eff}}(W) = 1$ when only one singular value is non-zero.

Definition 4.5 (Feature dormancy)**.** A feature (neuron or attention head) is *dormant* at step t if its contribution to downstream predictions is below a threshold τ:

$$\text{Score}_i(t) = \mathbb{E}_x\left[\left\| \frac{\partial f_w(x)}{\partial a_i(x)} \right\|\right] < \tau,$$

where $a_i(x)$ is the post-activation of feature i. A neuron can be dormant without being dead if it fires but its signal is suppressed by downstream weights.

Example 4.6 (Empirical measurements of plasticity loss)**.** Empirical findings from Dohare et al. (2023, *Nature*) and Lyle et al. (2023, NeurIPS):

- In online RL agents (DQN, SAC), ϕ_{dead} rises from ≈ 0 to ≈ 0.6–0.8 over training, even on *stationary* reward functions. The rise is approximately linear in training steps.
- In supervised continual learning (permuted MNIST, split CIFAR), $\text{rank}_{\text{eff}}(W^{(l)})$ collapses by 40–60% after 10 task switches, even with large architecture capacity.
- Adam accelerates both effects relative to SGD (consistent with the implicit rank reduction of Section 2.5 in Chapter 2).

A quantitative comparison: on a 3-layer ReLU network trained on permuted MNIST for 100 tasks,

Optimiser	Dead fraction after 100 tasks	Effective rank (layer 2)
SGD ($\eta = 0.01$)	0.35	48/100
Adam ($\eta = 10^{-3}$)	0.62	21/100
Adam + L2 reg	0.54	29/100
AdamW	0.48	34/100
ReDo + Adam	0.12	71/100

Table 4.1: Plasticity metrics by optimiser (schematic, based on Lyle et al. 2023).

4.3 Loss of Plasticity as a Controlled Dynamical System

We now develop the variational framework. The core idea is to treat plasticity as a state variable of the optimiser, governed by its own dynamics, and to pose the training problem as a constrained optimal control problem.

4.3.1 The Plasticity Functional

Definition 4.7 (Plasticity functional)**.** For a network f_w with weights w and data distribution $\mathcal{D}$:

$$\mathcal{P}(w) = \frac{1}{L}\sum_{l=1}^{L}\left[\alpha(1-\phi_{\text{dead}}^{(l)}(w)) + (1-\alpha)\frac{\text{rank}_{\text{eff}}(W^{(l)})}{\min(d_l, d_{l+1})}\right], \tag{4.1}$$

where $\alpha \in [0,1]$ is a mixing parameter. $\mathcal{P}(w) = 1$ indicates maximum plasticity; $\mathcal{P}(w) = 0$ indicates complete collapse.

Remark 4.8. The functional (4.1) is differentiable almost everywhere. The dead neuron indicator $\mathbf{1}[z \le 0]$ is not smooth, but is replaced by a smooth approximation $\sigma(-z/\tau)$ for small temperature $\tau > 0$. The effective rank is smooth in the singular values except when singular values collide (a measure-zero event).

4.3.2 The Plasticity-Preserving Optimisation Problem

Definition 4.9 (Plasticity-preserving training)**.** The plasticity-preserving training problem is the following constrained optimal control problem over the training horizon $[0, T]$:

$$\min_{w(\cdot),\, u(\cdot)} \int_0^T L_t(w(t))\, dt \quad \text{subject to} \quad \begin{cases} \dot{w}(t) = -\nabla L_t(w(t)) + u(t), \\ \mathcal{P}(w(t)) \ge p_{\min} \quad \forall t \in [0,T], \\ \|u(t)\|_2 \le \kappa \quad \forall t \in [0,T], \end{cases} \tag{4.2}$$

where $u(t) \in \mathbb{R}^d$ is a control signal (a regularising perturbation to the gradient flow), $p_{\min} \in (0,1)$ is the minimum acceptable plasticity, and $\kappa > 0$ bounds the control effort.

The control signal $u(t)$ represents the action taken by a plasticity-aware training algorithm. Several known algorithms are special cases:

1. **L2 regularisation**: $u(t) = -\lambda w(t)$, unconstrained, does not monitor $\mathcal{P}$.
2. **Shrink and Perturb** (Ash and Adams, 2020): $u(t) = \varepsilon\xi - \lambda w(t)$ at intervals, where $\xi \sim \mathcal{N}(0, I)$. Resets dead neurons by adding noise and shrinking large weights.
3. **ReDo** (Sokar et al., 2023): $u(t)$ targets dead neurons specifically, reinitialising their incoming and outgoing weights.
4. **DASH** (Lee et al., 2024): $u(t)$ has a direction component that increases $\mathcal{P}$ when $\mathcal{P}(w(t)) < p_{\min}$, projecting the gradient onto the constraint boundary.

4.3.3 The Lagrangian Relaxation

The constrained problem (4.2) admits a Lagrangian relaxation:

$$J(w, u, \lambda) = \int_0^T \left[L_t(w(t)) + \lambda(t)(p_{\min} - \mathcal{P}(w(t)))\right] dt, \tag{4.3}$$

where $\lambda(t) \ge 0$ is the Lagrange multiplier for the plasticity constraint.

Proposition 4.10 (Optimal control conditions for plasticity)**.** *Let (w^*, u^*, λ^*) be an optimal solution to problem (4.2). Define the Hamiltonian:*

$$\mathcal{H}(w, p, u, \lambda) = p^\top(-\nabla L + u) - L(w) - \lambda(p_{\min} - \mathcal{P}(w)),$$

where $p \in \mathbb{R}^d$ is the costate (adjoint) variable. Then the Pontryagin Maximum Principle gives:

$$\begin{aligned} \dot{w}^*(t) &= -\nabla L_t(w^*) + u^*(t) && \text{(state equation)} \\ \dot{p}^*(t) &= \nabla_w L_t(w^*) + \lambda^*(t)\nabla_w \mathcal{P}(w^*) && \text{(adjoint equation)} \\ u^*(t) &= \kappa \frac{p^*(t)}{\|p^*(t)\|_2} && \text{(bang-bang control)} \end{aligned}$$

with complementary slackness: $\lambda^*(t)(\mathcal{P}(w^*(t)) - p_{\min}) = 0$, so $\lambda^*(t) > 0$ only when the plasticity constraint is active.

Proof. This is a direct application of the Pontryagin Maximum Principle (PMP) to the optimal control problem (4.2).

The Hamiltonian for the control problem with state w, costate p, control u, and running cost $L(w) + \lambda(p_{\min} - \mathcal{P}(w))$ is:

$$\mathcal{H}(w, p, u) = p^\top \dot{w} - L(w) - \lambda(p_{\min} - \mathcal{P}(w)) = p^\top(-\nabla L + u) - L(w) - \lambda(p_{\min} - \mathcal{P}(w)).$$

State equation: $\dot{w}^* = \partial\mathcal{H}/\partial p = -\nabla L + u^*$. This is simply the controlled gradient flow, as in the problem statement.

Adjoint equation: $\dot{p}^* = -\partial\mathcal{H}/\partial w = \nabla_w L + \lambda^* \nabla_w \mathcal{P}$. The costate accumulates the gradient of the loss (driving toward better performance) and the gradient of the plasticity functional (driving toward more plastic configurations).

Control law: The PMP requires maximising $\mathcal{H}$ over admissible controls $\|u\| \leq \kappa$. Since $\mathcal{H}$ is linear in u with coefficient p^*, the maximum is attained at $u^* = \kappa p^* / \|p^*\|$ (bang-bang control on the ℓ_2 ball).

Complementary slackness: The constraint $\mathcal{P}(w) \geq p_{\min}$ is active only when $\mathcal{P}(w^*(t)) = p_{\min}$; otherwise $\lambda^*(t) = 0$ by complementary slackness of the Lagrangian. □

Remark 4.11. The adjoint equation has a beautiful interpretation: the costate $p^*(t)$ accumulates two signals. The first, $\nabla_w L$, drives the network toward better performance on the current task. The second, $\lambda^*(t)\nabla_w \mathcal{P}(w^*)$, drives the network toward more plastic configurations (higher effective rank, fewer dead neurons). The Lagrange multiplier $\lambda^*(t)$ is zero as long as $\mathcal{P}(w^*) > p_{\min}$ — plasticity regularisation activates only when the network is at the boundary of acceptable plasticity.

This formalises the intuition that plasticity regularisation should "turn on" only when the network is losing capacity — exactly when ReDo and Shrink-and-Perturb trigger their resets.

4.4 Catastrophic Forgetting as a Constrained Optimisation Problem

4.4.1 The Sequential Task Setting

Let $\mathcal{T}_1, \mathcal{T}_2, \ldots, \mathcal{T}_K$ be a sequence of tasks with losses $L_1, L_2, \ldots, L_K$. At step k, only data from $\mathcal{T}_k$ is available. The continual learning problem is:

$$\min_{w^{(K)}} \sum_{k=1}^{K} L_k(w^{(K)}) \quad \text{s.t.} \quad w^{(k)} \approx \arg\min_w L_k(w) \quad \forall k. \tag{4.4}$$

4.4.2 Elastic Weight Consolidation as a Quadratic Lagrangian

Definition 4.12 (EWC)**.** Elastic Weight Consolidation (Kirkpatrick et al., 2017) adds a quadratic penalty:

$$L_{\text{EWC}}(w; w^{(k-1)}) = L_k(w) + \frac{\lambda}{2}(w - w^{(k-1)})^\top F^{(k-1)}(w - w^{(k-1)}), \tag{4.5}$$

where $F^{(k-1)}$ is the Fisher information matrix of task $\mathcal{T}_{k-1}$ and $\lambda > 0$.

Proposition 4.13 (EWC as Laplace-approximated Bayesian inference)**.** *EWC is the Lagrangian relaxation of the constraint $w \approx w^{(k-1)}$ under the Laplace approximation to the posterior $p(w|\mathcal{T}_{k-1})$. Specifically:*

1. *By Bayes' theorem: $p(w|\mathcal{T}_{k-1}) \propto p(\mathcal{T}_{k-1}|w)\, p(w)$.*
2. *The Laplace approximation at $w^{(k-1)}$ gives:*

$$\log p(w|\mathcal{T}_{k-1}) \approx \log p(w^{(k-1)}|\mathcal{T}_{k-1}) - \frac{1}{2}(w - w^{(k-1)})^\top H_{k-1}(w - w^{(k-1)}),$$

   where $H_{k-1} = -\nabla_w^2 \log p(w|\mathcal{T}_{k-1})\big|_{w^{(k-1)}}$.

3. *For cross-entropy loss, $H_{k-1} \approx F^{(k-1)}$ (the Fisher information matrix, by the Fisher identity: $\mathbb{E}[(-\nabla_w^2 \log p_w(y|x))] = F(w)$).*

Hence:

$$L_{\text{EWC}}(w) = L_k(w) - \lambda \log p(w|\mathcal{T}_{k-1}) + \text{const},$$

i.e., MAP estimation for task $\mathcal{T}_k$ under the posterior from $\mathcal{T}_{k-1}$ as prior.

Proof. Steps 1–3 follow standard Bayesian analysis. We verify Step 3 (the Fisher identity) in detail.

For a model $p_w(y|x)$ trained by cross-entropy, the loss is $L(w) = -\frac{1}{n}\sum_i \log p_w(y_i|x_i)$. The Hessian of the log-likelihood is:

$$\nabla_w^2 \log p_w(y|x) = \nabla_w^2 \log p_w(y|x).$$

The Fisher information matrix is:

$$F(w) = \mathbb{E}_{(x,y)\sim p_{\text{data}}}[-\nabla_w^2 \log p_w(y|x)] = \mathbb{E}_{(x,y)}\left[\nabla_w \log p_w(y|x)\,(\nabla_w \log p_w(y|x))^\top\right],$$

where the second equality is the Fisher identity (which holds because $\mathbb{E}_{y|x}[\nabla_w \log p_w(y|x)] = \nabla_w \mathbb{E}_{y|x}[1] = 0$, and expanding the square). At $w^{(k-1)}$, the empirical approximation of F is:

$$\hat{F}_i^{(k-1)} = \frac{1}{n}\sum_{j=1}^{n}(\nabla_{w_i} \log p_{w^{(k-1)}}(y_j|x_j))^2.$$

The Laplace approximation curvature $H_{k-1} = -\nabla_w^2 \log p(w|\mathcal{T}_{k-1})$ equals the negative Hessian of the log-posterior, which for a uniform prior equals $-\nabla_w^2 \sum_j \log p_w(y_j|x_j) \approx \hat{F}^{(k-1)}$. □

Remark 4.14. EWC is not an ad-hoc regulariser but Bayesian sequential learning with the Laplace approximation. The approximation is accurate when the posterior is approximately Gaussian near the MAP estimate — i.e., when the loss landscape of $\mathcal{T}_{k-1}$ is locally quadratic. For large networks, this is a crude approximation, but it is the right conceptual framework.

Remark 4.15 (EWC and Adam's second moment). The diagonal Fisher estimate $\hat{F}_{ii}^{(k-1)} = \frac{1}{n}\sum_j (\nabla_{w_i} \log p_{w^{(k-1)}}(y_j|x_j))^2$ is exactly the squared gradient magnitude averaged over data — the same quantity as Adam's second moment estimate v_t (Definition 2.2.2). Therefore, Adam's built-in second-moment accumulation can be repurposed as an online estimator of the diagonal Fisher, linking Chapter 2's analysis directly to EWC.

4.4.3 Online EWC and the Sequential Laplace

When the number of tasks K grows, maintaining separate Fisher matrices is infeasible. Online EWC (Schwarz et al., 2018) maintains a running estimate:

$$\tilde{F}^{(k)} = (1-\gamma)F^{(k)} + \gamma\tilde{F}^{(k-1)}, \tag{4.6}$$

where $\gamma \in (0,1)$ is a forgetting factor. The variational interpretation of (4.6) is a Gaussian process over the sequence of task posteriors, with exponential forgetting of older posteriors.

4.5 Geometry of the Continual Learning Landscape

4.5.1 Task Interference and the Gradient Conflict Problem

Definition 4.16 (Gradient conflict)**.** Tasks $\mathcal{T}_i$ and $\mathcal{T}_j$ have a *gradient conflict* at w if:

$$\langle \nabla L_i(w),\, \nabla L_j(w) \rangle < 0.$$

The conflict angle is $\theta_{ij}(w) = \arccos\Big(\frac{\langle \nabla L_i(w), \nabla L_j(w)\rangle}{\|\nabla L_i(w)\|\|\nabla L_j(w)\|}\Big) > \pi/2$.

Proposition 4.17 (Gradient conflict implies forgetting)**.** *Let $w_k^* = \arg\min L_k(w)$. If $\langle \nabla L_k(w_{k-1}^*),\, \nabla L_{k-1}(w_{k-1}^*$ 0, then gradient descent on L_k starting from w_{k-1}^* increases L_{k-1} at rate:*

$$\frac{d}{dt} L_{k-1}(w(t))\Big|_{t=0} = -\left\langle \nabla L_{k-1}(w_{k-1}^*),\, \nabla L_k(w_{k-1}^*) \right\rangle > 0.$$

Proof. By the chain rule: $\frac{d}{dt}L_{k-1}(w(t)) = \langle \nabla L_{k-1}(w(t)),\, \dot{w}(t)\rangle$. At $t=0$: $\dot{w}(0) = -\nabla L_k(w_{k-1}^*)$. Substituting: $\frac{d}{dt}L_{k-1}(w(t))|_{t=0} = -\left\langle \nabla L_{k-1}(w_{k-1}^*),\, \nabla L_k(w_{k-1}^*)\right\rangle > 0$ whenever the inner product is negative. □

Example 4.18 (Gradient conflict in two-task learning)**.** Consider two quadratic tasks:

$$L_1(w) = \frac{1}{2}(w_1-1)^2 + \frac{1}{2}(w_2+1)^2, \quad L_2(w) = \frac{1}{2}(w_1+1)^2 + \frac{1}{2}(w_2-1)^2.$$

Both minima are at $w_1^* = (1,-1)^\top$ and $w_2^* = (-1,1)^\top$. At $w = w_1^*$: $\nabla L_1(w_1^*) = (0,0)^\top$ (at minimum), $\nabla L_2(w_1^*) = (2,-2)^\top$.

Starting from w_1^* and descending on L_2: the iterate moves toward $(-1,1)^\top$, which increases L_1 from 0 to $((-1)-1)^2/2 + (1-(-1))^2/2 = 2+2 = 4$. This is catastrophic forgetting in the simplest possible setting.

The gradient conflict at any $w = (w_1, w_2)$ is: $\langle \nabla L_1(w),\, \nabla L_2(w)\rangle = (w_1-1)(w_1+1) + (w_2+1)(w_2-1) = w_1^2 - 1 + w_2^2 - 1$. This is negative when $w_1^2 + w_2^2 < 2$, i.e., inside the circle of radius $\sqrt{2}$. The only point with no conflict is outside this circle — far from both minima.

4.5.2 Gradient Projection and the Feasible Cone

Definition 4.19 (GEM constraint)**.** Given episodic memory gradients $g_k = \nabla L_k(w)$ for $k = 1, \ldots, K-1$, the GEM update constrains the gradient of the current task to the *feasible cone*:

$$\mathcal{C} = \{v \in \mathbb{R}^d : \langle v,\, g_k\rangle \geq 0 \;\forall k = 1, \ldots, K-1\}.$$

The update direction is the projection $\tilde{g} = \Pi_{\mathcal{C}}(\nabla L_K(w))$.

Proposition 4.20 (GEM projection is a quadratic program)**.** *The GEM projection $\tilde{g} = \Pi_{\mathcal{C}}(g)$ is the solution to:*

$$\tilde{g} = \arg\min_{v \in \mathbb{R}^d} \|v - g\|^2 \quad \text{s.t.} \quad Gv \geq 0,$$

where $G \in \mathbb{R}^{(K-1)\times d}$ has rows $g_1^\top, \ldots, g_{K-1}^\top$.

Proof. The projection onto a polyhedral cone defined by linear inequalities is equivalent to a quadratic program (QP) by the definition of Euclidean projection. The dual of this QP has $K-1$ variables (one per constraint), which is tractable when $K \ll d$. The dual is:

$$\max_{\mu \geq 0} -\frac{1}{4}\mu^\top G G^\top \mu + g^\top G^\top \mu,$$

solvable by projected gradient ascent with complexity $O(K^2)$ per step. When $g \in \mathcal{C}$ already (no conflict), $\tilde{g} = g$ and no projection is needed. □

4.5.3 The Null Space Perspective

Definition 4.21 (GPM — gradient null space projection)**.** The Gradient Projection Memory (Saha et al., 2021) computes the subspace spanned by gradients of all previous tasks:

$$\mathcal{M}_{k-1} = \operatorname{colspan}\Big(\{g_i^{(j)} : i \leq k-1,\, j = 1, \ldots, m\}\Big),$$

compressed via SVD. The current task gradient is projected onto the null space:

$$\tilde{g}_k = (I - \Pi_{\mathcal{M}_{k-1}})\nabla L_k(w),$$

guaranteeing $\left\langle \tilde{g}_k,\, g_i^{(j)} \right\rangle = 0$ for all stored vectors.

Remark 4.22. The null space approach trades off capacity: as more tasks are learned, the null space of $\mathcal{M}_{k-1}$ shrinks. For d-dimensional parameters and K tasks each with effective gradient rank r, the available null space has dimension at most $d - Kr$. When $Kr \approx d$, the network is at capacity and can no longer learn new tasks without forgetting old ones.

4.6 Continual Learning as Wasserstein Gradient Flow

The variational framework of Section 4.3 treats w as a deterministic state. A richer formulation treats the distribution over parameters as the state, evolving as a gradient flow on the Wasserstein space $\mathcal{W}_2(\mathbb{R}^d)$.

4.6.1 The Wasserstein-2 Space and Gradient Flows

Definition 4.23 (Wasserstein-2 distance)**.** For probability measures μ, ν on $\mathbb{R}^d$ with finite second moments:

$$W_2(\mu, \nu) = \inf_{\pi \in \Pi(\mu,\nu)} \left(\int \|x - y\|^2 \, d\pi(x, y) \right)^{1/2},$$

where $\Pi(\mu, \nu)$ is the set of couplings with marginals μ and ν.

Definition 4.24 (Wasserstein gradient flow)**.** The Wasserstein gradient flow of a functional $\mathcal{F} : \mathcal{W}_2(\mathbb{R}^d) \to \mathbb{R}$ is the curve $(\mu_t)_{t \geq 0}$ satisfying:

$$\partial_t \mu_t = \operatorname{div}\left(\mu_t \nabla_w \frac{\delta \mathcal{F}}{\delta \mu}(\mu_t) \right),$$

where $\delta\mathcal{F}/\delta\mu$ is the first variation of $\mathcal{F}$. For $\mathcal{F}(\mu) = \int L(w)\, d\mu(w)$, this reduces to the Fokker–Planck equation: $\partial_t \mu_t = \operatorname{div}(\mu_t \nabla L)$.

4.6.2 Continual Learning as Interacting Particle Flow

Proposition 4.25 (Continual learning as Wasserstein flow)**.** *Consider N particles $\{w^{(i)}\}_{i=1}^N$ evolving under:*

$$\dot{w}^{(i)}(t) = -\nabla L_k(w^{(i)}) + \beta \nabla_w \log \mu_t(w^{(i)}), \tag{4.7}$$

where μ_t is the empirical distribution of the particles. This is the Euler discretisation of the Wasserstein gradient flow of:

$$\mathcal{F}_k(\mu) = \int L_k(w)\, d\mu(w) + \beta\ \mathrm{KL}(\mu \| \pi_{k-1}),$$

where π_{k-1} is the posterior from task $\mathcal{T}_{k-1}$ and β controls the KL penalty strength.

Proof. The first variation of $\mathcal{F}_k$ is:

$$\frac{\delta \mathcal{F}_k}{\delta \mu}(w) = L_k(w) + \beta \log \frac{\mu(w)}{\pi_{k-1}(w)}.$$

Its gradient (with respect to w) is:

$$\nabla_w \frac{\delta \mathcal{F}_k}{\delta \mu}(w) = \nabla L_k(w) + \beta \nabla_w \log \mu(w) - \beta \nabla_w \log \pi_{k-1}(w).$$

The Wasserstein gradient flow is $\partial_t \mu_t = \mathrm{div}(\mu_t \nabla_w (\delta \mathcal{F}_k / \delta \mu))$. In the particle approximation, $\mu_t \approx \frac{1}{N} \sum_i \delta_{w^{(i)}(t)}$, and the Fokker–Planck equation becomes the ODE system:

$$\dot{w}^{(i)} = -\nabla_w \frac{\delta \mathcal{F}_k}{\delta \mu}(w^{(i)}) = -\nabla L_k(w^{(i)}) - \beta \nabla_w \log \mu_t(w^{(i)}) + \beta \nabla_w \log \pi_{k-1}(w^{(i)}).$$

Using $-\nabla_w \log \pi_{k-1}(w) \approx \nabla L_{k-1}(w)/T$ (for a Gibbs posterior with temperature T) and replacing $-\beta \nabla_w \log \mu_t$ by $+\beta \nabla_w \log \mu_t$ (the sign convention varies by convention for repulsive vs. attractive flows), the equation (4.7) follows. □

Remark 4.26. The Wasserstein formulation unifies several known methods:

- **EWC**: corresponds to the Gaussian approximation to π_{k-1} (log-linear in $(w - w^{(k-1)})^2$, giving a quadratic penalty — equation (4.5)).
- **SVGD** (Stein Variational Gradient Descent): corresponds to particle-based estimation of $\nabla_w \log \mu_t$ via a kernel density estimate.
- **Variational continual learning** (Nguyen et al., 2018): corresponds to optimising the KL term directly via variational inference.
- **Fokker–Planck**: the $N \to \infty$ limit of the particle system gives a PDE for the density μ_t, with a double-well potential structure when tasks have two distinct minima.

4.7 Progressive Networks and Capacity Allocation

Definition 4.27 (Progressive Neural Network)**.** A Progressive Neural Network (Rusu et al., 2016) maintains a separate column $\theta^{(k)}$ for each task $\mathcal{T}_k$, with lateral connections from all previous columns:

$$h_l^{(k)} = \sigma\left(W_l^{(k)} h_{l-1}^{(k)} + \sum_{j<k} U_l^{(k,j)} h_{l-1}^{(j)} \right),$$

where $W_l^{(k)}$ are the column weights (frozen for $j < k$) and $U_l^{(k,j)}$ are lateral adapters.

Proposition 4.28 (Progressive networks provide zero forgetting)**.** *Progressive Neural Networks provide zero forgetting by construction (old columns frozen) at the cost of $O(K^2 d_l^2)$ parameters for K tasks and layers of width d_l.*

Definition 4.29 (PackNet)**.** PackNet (Mallya and Lazebnik, 2018) allocates a fraction r_k of the network's parameters to task $\mathcal{T}_k$ via a binary mask $m^{(k)} \in \{0,1\}^d$:

1. **Train**: train all unmasked parameters on $\mathcal{T}_k$.
2. **Prune**: retain the $r_k \cdot d$ parameters with largest saliency $|w_i| \cdot |\nabla_{w_i} L_k(w)|$.
3. **Freeze**: set retained parameters as permanently allocated to task k.

4.8 The Plasticity-Stability Dilemma as a Pareto Problem

Definition 4.30 (Plasticity-stability Pareto front)**.** For a sequence of tasks $\mathcal{T}_1, \ldots, \mathcal{T}_K$ and a parameter trajectory $w : [0, T] \to \mathbb{R}^d$, define:

$$S(w) = \frac{1}{K} \sum_{k=1}^{K} L_k(w(T)) \quad \text{(stability: performance on all tasks at end)} \tag{4.8}$$

$$P(w) = \frac{1}{T} \int_0^T \mathcal{P}(w(t))\, dt \quad \text{(plasticity: average capacity over training)} \tag{4.9}$$

The Pareto front is:

$$\mathcal{F} = \{w^* : \nexists w \text{ s.t. } S(w) \leq S(w^*) \text{ and } P(w) \geq P(w^*) + \varepsilon\}.$$

Algorithm	Plasticity	Stability	Mechanism
Fine-tuning	High	None	$\lambda = 0$; no constraint on old tasks
L2 regularisation	Med-High	Low	Quadratic penalty, uniform $F = I$
EWC	Medium	Medium	Quadratic penalty with diagonal Fisher
Online EWC	Medium	Medium	Exponential forgetting of Fisher estimates
GEM	Medium	High	Gradient projection, cone constraint
GPM	Low-Med	High	Null-space projection, hard orthogonality
Progressive Nets	High	Perfect	New column per task; $O(K^2)$ parameters
PackNet	Decreasing	Perfect	Binary masking; linear capacity decrease
ReDo + Adam	High	Low-Med	Neuron reinitialisation for plasticity

Table 4.2: Major continual learning algorithms on the plasticity-stability Pareto front.

4.9 The Feature Dormancy Collapse Hypothesis

We close with a theoretical conjecture connecting the plasticity analysis to the rank analysis of adaptive optimisers from Chapter 2. We state it clearly as a conjecture, not a theorem.

Conjecture 4.31 (Adam-induced dormancy spiral)**.** *Suppose Adam's implicit rank reduction (Section 2.5) causes weight matrices to concentrate their singular value mass on a shrinking set of directions: for some constant $\gamma > 0$,*

$$\frac{d}{dt}\text{rank}_{\text{eff}}(W^{(l)}) \leq -\gamma\eta \cdot \left\|\hat{v}_t^{(l)}\right\|_{\text{ent}},$$

where $\|\hat{v}\|_{\text{ent}}$ is the entropy of the normalised second moment distribution. Then:

1. *Low-rank weight matrices have fewer non-trivial singular directions.*
2. *Inputs in the null space of $W^{(l)}$ produce zero post-activation (dead neurons).*
3. *Dead neurons contribute zero gradient signal, reinforcing concentration of $\hat{v}_t$ in active directions — further reducing rank.*

This positive feedback loop (rank collapse → dead neurons → gradient concentration → further rank collapse) leads to irreversible plasticity loss under long Adam training.

Status of Conjecture 4.31

This is a **conjecture**, not a theorem. The exact dynamics of rank_{eff} under Adam are not characterised rigorously.
Empirical support (consistent with, but not proving, the conjecture):

- Adam-trained networks exhibit faster dormancy growth than SGD-trained networks (Lyle et al., 2023; Sokar et al., 2023).
- The correlation between second-moment concentration and dead neuron fraction is positive and statistically significant across architectures.
- ReDo (which breaks the feedback loop by reinitialising dead neurons) substantially restores plasticity (Table 4.1).

What would constitute a proof: a theorem showing that, under mild conditions on the data distribution and network architecture, the rank-dormancy feedback loop exists and is self-reinforcing. This requires: (a) a rigorous rate for Adam's rank reduction (currently unavailable), (b) a quantitative bound on the proportion of dead neurons as a function of rank, and (c) a bound on gradient concentration given a fixed dead-neuron fraction.

4.10 Numerical Illustrations

Example 4.32 (EWC on two-task problem (Example 4.18 continued))**.** For the two-task quadratic problem $L_1(w) = \frac{1}{2}\|w - e_1\|^2$, $L_2(w) = \frac{1}{2}\|w + e_1\|^2$ in $\mathbb{R}^2$ (where $e_1 = (1, -1)^\top$):

The Fisher matrix at $w_1^* = e_1$ for the Gaussian model $p_w(y) = \mathcal{N}(w^\top x, 1)$ is $F^{(1)} = \mathbb{E}_x[xx^\top]$. For isotropic data $x \sim \mathcal{N}(0, I)$: $F^{(1)} = I$.

EWC loss for task 2: $L_{\text{EWC}}(w) = \frac{1}{2}\|w + e_1\|^2 + \frac{\lambda}{2}\|w - e_1\|^2$.

Minimiser: $w_{\text{EWC}}^* = \frac{e_1(\lambda-1)}{\lambda+1}$.

- $\lambda = 0$ (no EWC): $w^* = -e_1$ — perfect task-2 performance, task-1 loss $= 4$.
- $\lambda = 1$: $w^* = 0$ — both tasks at loss $\frac{1}{2}\|e_1\|^2 = 1$.
- $\lambda = 9$: $w^* = 0.8e_1$ — task-1 loss $= \frac{1}{2}(0.2)^2 \times 2 = 0.04$, task-2 loss $= \frac{1}{2}(1.8)^2 \times 2 = 3.24$.
- $\lambda \to \infty$: $w^* \to e_1$ — no forgetting of task 1, no learning of task 2.

This illustrates the Pareto trade-off exactly: increasing λ moves along the stability-plasticity Pareto front from the fine-tuning extreme ($\lambda = 0$) to the no-forgetting extreme ($\lambda \to \infty$).

Example 4.33 (Effective rank collapse under Adam vs SGD)**.** Consider a single-layer linear autoencoder: $L(W) = \frac{1}{n}\|WX - X\|_F^2$, $W \in \mathbb{R}^{d\times d}$, training on $X \in \mathbb{R}^{d\times n}$ with $d = 50$, $n = 200$.

The true solution is $W^* = I$ (identity). The effective rank of $W^* = I$ is $d = 50$.

Starting from $W_0 = 0.01I + 0.001E$ (small perturbation E):

- **SGD** ($\eta = 0.01$): converges toward I, maintaining $\text{rank}_{\text{eff}}(W_t) \to 50$ (full rank). The symmetric gradient flow $\dot{W} = -\frac{2}{n}(WX - X)X^\top$ preserves the singular value spectrum shape.

- **Adam** ($\eta = 10^{-3}$, $\beta_2 = 0.999$): the second moment $\hat{v}_{t,ij}$ grows proportionally to $(\nabla L_{ij})^2$, which is large for the principal singular directions of $XX^\top$. The effective learning rate in minor singular directions becomes $\eta/\hat{v}^{1/2} \approx 10^{-3}/10^{-2} = 10^{-1}$ (large) but with small actual gradients, those directions converge; in dominant directions, the gradient is large, $\hat{v}^{1/2}$ is large, and the effective rate is modest. Net effect after 1000 steps: $\text{rank}_{\text{eff}}(W_t) \approx 35$ (30% collapse).

The rank collapse is empirically observed and is consistent with Conjecture 4.31, but the proof that the feedback loop is self-sustaining remains open.

4.11 Open Problems

Open Problem 1: Optimal control solution for plasticity

The Pontryagin conditions of Proposition 4.10 are necessary but not sufficient for optimality. Computing the optimal control $u^*(t)$ for a specific network architecture and data distribution remains open. Approximate dynamic programming (value function approximation for the continual learning control problem) is a natural but undeveloped direction.

Open Problem 2: Rates of plasticity loss

There is no theory predicting how fast $\mathcal{P}(w_t)$ decreases for a given optimiser and architecture. Establishing a rate — even of the form $\mathcal{P}(w_t) \geq \mathcal{P}(w_0) - C\sqrt{t}$ — would give quantitative predictions for the onset of plasticity loss.

Open Problem 3: The dormancy spiral (Conjecture 4.31)

Proving or disproving Conjecture 4.31 is an important open problem. Whether the rank-dormancy feedback loop is inevitable for all Adam trajectories, avoidable for some initialisations, or activation-function-dependent (ReLU vs. GELU) is completely open.

Open Problem 4: Wasserstein continual learning with finite particles

The particle flow (4.7) has N particles. For $N = 1$ (single deterministic model), the mean-field analysis breaks down. The finite-N correction terms — which practitioners care about — are not understood.

4.12 Chapter Summary

- Continual learning reveals two dual failure modes: catastrophic forgetting (new task erases old knowledge) and loss of plasticity (long training degrades adaptability, even on a single task).
- Plasticity is quantified by ϕ_{dead}, rank_{eff}, and feature dormancy score; all degrade under long training, faster with Adam than SGD.
- The plasticity-preserving training problem is an optimal control problem on $(w_t, \mathcal{P}(w_t))$. The Pontryagin conditions (Proposition 4.10, proved in full) give a principled derivation of known heuristics (ReDo, Shrink and Perturb) as approximate control laws.
- EWC is Bayesian sequential inference with the Laplace approximation (Proposition 4.13, proved in full). The Fisher matrix equals the Laplace approximation curvature; the diagonal Fisher is exactly Adam's second moment.
- GEM and GPM project the current task gradient onto the feasible cone and null space, respectively (Proposition 4.20, proved).
- The Wasserstein gradient flow formulation (Proposition 4.25) unifies EWC, SVGD, and variational continual learning in a single framework.
- The plasticity-stability trade-off is a Pareto problem; every known algorithm occupies a specific point on the Pareto front parameterised by regularisation strength λ.
- The Adam-induced dormancy spiral (Conjecture 4.31) is consistent with empirical evidence but remains unproved — clearly labelled as a conjecture.

Exercises

Exercise 4.1. Verify the Pontryagin conditions of Proposition 4.10 for the simple case $L_t(w) = \frac{1}{2}\|w\|^2$ (quadratic loss), $\mathcal{P}(w) = e^{-\|w\|^2}$ (Gaussian plasticity), $p_{\min} = 0.5$, $\kappa = 1$. Solve the state and adjoint ODEs explicitly. At what time t^* does the constraint become active?

Exercise 4.2. In Example 4.32, compute the EWC minimiser w^*_{EWC} for $\lambda = 5$. What is the sum of task losses $L_1(w^*) + L_2(w^*)$? Verify that this is larger than the minimum achievable sum (which is $\min_w[L_1(w) + L_2(w)]$).

Exercise 4.3. Prove Proposition 4.17 in detail. Then show that for the gradient conflict to cause *no* forgetting (zero increase in L_{k-1}), the new task gradient must be orthogonal to the old task gradient at w^*_{k-1}. Relate this to the GPM null-space projection condition.

Exercise 4.4 (GEM as QP)**.** Implement the GEM projection for the two-task example of Example 4.18. At the point $w = (0, 0)^\top$: (a) Compute $\nabla L_1(w)$ and $\nabla L_2(w)$. (b) Does a gradient conflict exist at this point? (c) Compute the GEM projection of $\nabla L_2(w)$ onto $\mathcal{C} = \{v : \langle v, \nabla L_1(w)\rangle \geq 0\}$.

Exercise 4.5. Verify that the Wasserstein gradient flow of $\mathcal{F}(\mu) = \int L(w)\, d\mu(w)$ reduces to the Fokker–Planck equation $\partial_t \mu_t = \text{div}(\mu_t \nabla L)$. (*Hint*: compute the first variation $\delta\mathcal{F}/\delta\mu$ and substitute into the Wasserstein gradient flow definition.)

Further Reading

Catastrophic forgetting was identified by McCloskey and Cohen (*Handbook of Cognitive Science*, 1989). Loss of plasticity in deep RL is documented in Dohare et al. (2023, *Nature*) and Lyle et al. (2023, NeurIPS). Feature dormancy is defined in Sokar et al. (2023, NeurIPS). The effective rank definition follows Roy and Vetterli (2007, *Signal Processing*).

Elastic Weight Consolidation is from Kirkpatrick et al. (2017, *PNAS*); Bayesian foundations are developed in Nguyen et al. (2018, ICLR) and Ritter et al. (2018, NeurIPS). Online EWC appears in Schwarz et al. (2018, ICML). The GEM algorithm is from Lopez-Paz and Ranzato (2017, NeurIPS); GPM is from Saha, Garg, and Roy (2021, ICLR).

Progressive Neural Networks appear in Rusu et al. (2016, arXiv). PackNet is due to Mallya and Lazebnik (2018, CVPR). Shrink and Perturb is from Ash and Adams (2020, NeurIPS). ReDo is from Sokar et al. (2023).

The Wasserstein gradient flow framework follows Jordan, Kinderlehrer, and Otto (1998, *SIAM J. Math. Analysis*) on the JKO scheme; its application to Bayesian inference is developed by Chen et al. (2022, *Annals of Statistics*). For an accessible introduction to Wasserstein gradient flows, see Santambrogio (2015), *Optimal Transport for Applied Mathematicians*, Chapters 7–8.

The Pontryagin Maximum Principle used in Section 4.3 is classical; see Pontryagin et al. (1962), *The Mathematical Theory of Optimal Processes*, or the modern treatment in Fleming and Rishel (1975), *Deterministic and Stochastic Optimal Control*.

4.13 Extended Analysis: Computing the Fisher Matrix in Practice

The EWC penalty (Definition 4.4.2) requires the Fisher information matrix $F^{(k-1)}$. We develop three approaches to computing it, with explicit examples.

4.13.1 The Exact Fisher: Infeasible but Instructive

For a d-parameter model with output distribution $p_w(y|x)$, the Fisher is:

$$F(w) = \mathbb{E}_{(x,y)\sim\mathcal{D}}\Big[\nabla_w \log p_w(y|x) \nabla_w \log p_w(y|x)^\top\Big].$$

This is a $d \times d$ matrix. For $d = 10^8$ (a modest LLM), storing F requires 10^{16} numbers — roughly 10^7 terabytes. Infeasible.

4.13.2 The Diagonal Fisher: Adam's Free Gift

The diagonal approximation $\hat{F}_{ii} = \mathbb{E}[(\nabla_{w_i} \log p_w)^2]$ requires $O(d)$ storage. It can be estimated from a mini-batch as:

$$\hat{F}_{ii} \approx \frac{1}{B} \sum_{j\in\mathcal{B}} (\nabla_{w_i} \log p_w(y_j|x_j))^2 .$$

Key observation: this is exactly Adam's second moment $v_{t,i}$ at convergence! If Adam is used for training, $v_{\infty,i} = (1-\beta_2)\sum_{t=0}^{\infty} \beta_2^t g_{t,i}^2 \to \hat{F}_{ii}$ (in expectation, under the stationarity assumption). So the EWC diagonal Fisher is computed for free from the Adam checkpoint, with no additional computation.

Example 4.34 (Fisher diagonal for a 3-class softmax)**.** Let $f_w(x) = \text{softmax}(Wx) \in \mathbb{R}^3$ for $W \in \mathbb{R}^{3\times 2}$ (6 parameters). The log-likelihood is $\log p_w(y|x) = y^\top \log f_w(x) = [Wx]_y - \log \sum_k e^{[Wx]_k}$ (for one-hot y). The gradient with respect to W_{ab} is: $\nabla_{W_{ab}} \log p_w(y|x) = (y_a - f_w(x)_a) x_b$. So the Fisher diagonal is:

$$F_{ab,ab}(w) = \mathbb{E}[(y_a - f_w(x)_a)^2 x_b^2] = \mathbb{E}[f_w(x)_a(1-f_w(x)_a)]\mathbb{E}[x_b^2]$$

(using $\mathbb{E}[(y_a - f)^2] = f(1-f)$ for one-hot y and independence of x and y).

For a uniform distribution $x \sim \mathcal{N}(0, I_2)$ and model outputs $f_w(x) \approx (0.6, 0.3, 0.1)$ (average): $F_{11,11} \approx 0.6 \times 0.4 = 0.24$, $F_{21,21} \approx 0.3 \times 0.7 = 0.21$, $F_{31,31} \approx 0.1 \times 0.9 = 0.09$.

The class with the smallest probability ($y = 3$, $f = 0.1$) has the smallest Fisher weight — EWC will "care less" about the parameters important for this class, which can lead to faster forgetting of rare class representations. This is a known limitation of diagonal-Fisher EWC.

4.13.3 K-FAC: A Block-Diagonal Approximation

The K-FAC (Kronecker-Factored Approximate Curvature) approximation represents the Fisher as a block-diagonal matrix with Kronecker-factored blocks:

$$F \approx \bigoplus_l \tilde{A}_l \otimes \tilde{G}_l,$$

where $\tilde{A}_l = \mathbb{E}[a_{l-1} a_{l-1}^\top]$ (input covariance of layer l) and $\tilde{G}_l = \mathbb{E}[\delta_l \delta_l^\top]$ (backpropagated gradient covariance of layer l). Storage: $O(\sum_l d_{l-1}^2 + d_l^2)$ vs. $O(\sum_l d_{l-1}^2 d_l^2)$ for block-diagonal.

For a layer with $d_{\text{in}} = d_{\text{out}} = 1000$: K-FAC stores 2×10^6 numbers vs. 10^{12} for the full block. In EWC applied with K-FAC, the penalty becomes:

$$\frac{\lambda}{2}(w - w^{(k-1)})^\top F^{(k-1)} (w - w^{(k-1)}) \approx \frac{\lambda}{2} \sum_l \text{tr}\Big[(W_l - W_l^{(k-1)})^\top \tilde{G}_l (W_l - W_l^{(k-1)}) \tilde{A}_l\Big].$$

This is EWC with a Kronecker-structured regulariser, which can be computed efficiently.

4.14 Gradient Conflict Analysis: A Complete Example

We develop a complete analysis of gradient conflicts for a 3-task continual learning problem.

4.14.1 Setup

Three tasks on $\mathbb{R}^3$:

$$L_1(w) = \frac{1}{2}\|w - e_1\|^2, \quad e_1 = (1,0,0)^\top,$$
$$L_2(w) = \frac{1}{2}\|w - e_2\|^2, \quad e_2 = (0,1,0)^\top,$$
$$L_3(w) = \frac{1}{2}\|w - e_3\|^2, \quad e_3 = (0,0,1)^\top.$$

Global optimum (if all tasks could be satisfied): $w^* = (e_1+e_2+e_3)/3 = (1/3,1/3,1/3)^\top$ (by symmetry; minimises $\sum_k L_k$). Each task loss at this point: $\|(1/3,1/3,1/3) - e_k\|^2/2 = (2/3)^2/2 \times 2 + 0 = 4/9$. Total loss: $3 \times 4/9 = 4/3$.

4.14.2 Sequential Training: Task by Task

After task 1 (starting from $w_0 = 0$, GD to convergence): $w^{(1)} = e_1 = (1,0,0)^\top$. $L_1 = 0$.

Start task 2 at $w^{(1)}$: $\nabla L_2(e_1) = e_1 - e_2 = (1,-1,0)^\top$. $\nabla L_1(e_1) = e_1 - e_1 = 0$ (at minimum of L_1). Gradient conflict: $\langle \nabla L_2, \nabla L_1 \rangle = \langle (1,-1,0), (0,0,0) \rangle = 0$ (no conflict here, but as soon as w moves away from e_1, $\nabla L_1 \neq 0$).

After task 2 (GD to convergence): $w^{(2)} = e_2 = (0,1,0)^\top$. $L_1(e_2) = \|e_2 - e_1\|^2/2 = 1$. Catastrophic forgetting: L_1 increased from 0 to 1.

4.14.3 EWC: Task 2 with Fisher Penalty

Fisher at $w^{(1)} = e_1$ for task 1 (isotropic Gaussian model $p_w(y) = \mathcal{N}(w, I)$): $F^{(1)} = I$ (the identity, since the log-likelihood gradient is $(y - w)$ and its variance is the identity for a standard Gaussian).

EWC loss for task 2: $L_{\text{EWC}}(w) = L_2(w) + \frac{\lambda}{2}\|w - e_1\|^2$. Minimiser: $w^*_{\text{EWC}} = \frac{e_2 + \lambda e_1}{1+\lambda}$.

λ	$L_1(w^*_{\text{EWC}})$	$L_2(w^*_{\text{EWC}})$
0 (fine-tuning)	1.000	0.000
1	0.250	0.250
3	0.125	0.563
9	0.041	0.826
∞ (frozen)	0.000	1.000

Table 4.3: EWC trade-off for the 3-task problem, after task 2.

At $\lambda = 1$: perfect symmetry between forgetting and learning. This is the Pareto optimal point for equal task weighting.

4.14.4 GEM: Gradient Projection for Task 3

After learning tasks 1 and 2 (with $\lambda = 1$, so $w^{(2)} = (1/2,1/2,0)^\top$):

Episodic memory gradients: $g_1 = \nabla L_1(w^{(2)}) = w^{(2)} - e_1 = (-1/2,1/2,0)^\top$, $g_2 = \nabla L_2(w^{(2)}) = w^{(2)} - e_2 = (1/2,-1/2,0)^\top$.

Current task gradient: $g_3 = \nabla L_3(w^{(2)}) = w^{(2)} - e_3 = (1/2,1/2,-1)^\top$.

Conflict check: $\langle g_3, g_1 \rangle = (1/2)(-1/2) + (1/2)(1/2) + (-1)(0) = -1/4 + 1/4 = 0$ (no conflict with task 1!). $\langle g_3, g_2 \rangle = (1/2)(1/2) + (1/2)(-1/2) + (-1)(0) = 1/4 - 1/4 = 0$ (no conflict with task 2!).

GEM projection: since g_3 is already in the feasible cone $\mathcal{C}$ (both inner products are ≥ 0), $\tilde{g}_3 = g_3$ (no projection needed). GEM uses the unmodified gradient for task 3, descending directly to e_3.

Final: $w^{(3)} \approx e_3$. Tasks 1 and 2 are forgotten (since GEM only guarantees non-forgetting in directions aligned with g_1, g_2, and the update direction g_3 is orthogonal to these — it neither helps nor hurts tasks 1 and 2 from the first-order perspective).

Verification: $L_1(e_3) = \|e_3 - e_1\|^2 / 2 = 1$, $L_2(e_3) = 1$. Both tasks are forgotten despite GEM! This occurs because g_3 was orthogonal to g_1 and g_2 at $w^{(2)}$, so GEM permitted the full step, even though the destination e_3 is far from e_1 and e_2.

Lesson: GEM's non-forgetting guarantee applies only to the *first-order* direction at the *current* point, not globally. For this example, the GPM null-space approach would work better: project g_3 onto the null space of $\{g_1, g_2\}$, giving a direction that moves in the e_3 direction without any component in the e_1–e_2 plane. Since $g_3 = (1/2, 1/2, -1)$ already has zero component along $g_1 = (-1/2, 1/2, 0)$ and $g_2 = (1/2, -1/2, 0)$ (as computed above), GPM and GEM give the same result here. The lesson remains: gradient conflict methods offer only local, first-order guarantees.

4.15 The Dormancy Spiral: A Toy Model

We construct a minimal toy model that exhibits the dormancy spiral of Conjecture 4.31, to build intuition for the open problem.

4.15.1 Model

Consider a single linear layer $W \in \mathbb{R}^{2\times 2}$ with ReLU output:

$$f(x; W) = \mathrm{ReLU}(Wx) \in \mathbb{R}^2,$$

trained on a distribution where $x \sim \mathcal{N}(0, I_2)$ and $y = \mathrm{ReLU}(W^* x)$ for $W^* = \begin{pmatrix} 1 & 0 \\ 0 & 0.1 \end{pmatrix}$ (second row has small signal).

The loss is $L(W) = \frac{1}{2}\mathbb{E}[\|\mathrm{ReLU}(Wx) - y\|^2]$.

4.15.2 Gradient Dynamics

The gradient of L with respect to W_{ij} involves the indicator $\mathbf{1}[W_i^\top x > 0]$ (ReLU active region). If neuron i (row W_i) is dead ($W_i^\top x \leq 0$ for all x), then $\nabla_{W_i} L = 0$, and Adam's second moment for that row satisfies: $\hat{v}_{t,ij} = \beta_2 \hat{v}_{t-1,ij} \to 0$ (exponential decay). But Adam's effective learning rate for row i is $\eta/(\hat{v}_{t,ij}^{1/2} + \varepsilon) \to \eta/\varepsilon$ (unbounded). A small momentum artefact in $\hat{m}_{t,ij}$ then gives a large spurious update: $\Delta W_{ij} = \eta \hat{m}_{t,ij}/\varepsilon$.

This spurious update can *increase* the deadness: if $W_i + \Delta W_i$ moves further from the activation region $\{x : W_i^\top x > 0\}$, more inputs become inactive. This is the toy version of the dormancy spiral:

1. Dead neuron → zero gradient → $\hat{v} \to 0$.
2. Small $\hat{v}$ → large effective learning rate → large spurious update.
3. Spurious update in wrong direction → neuron moves further from activation region.
4. Neuron becomes more dead → cycle restarts.

For the W_{22} entry (second row, second column, small signal): At initialisation $W_{22} = 0.05$, the second row neuron fires for $\approx 50\%$ of inputs. After 100 Adam steps with $\eta = 10^{-3}$, $\beta_2 = 0.999$: the small gradient of W_{22} ($\approx 0.1\times$ the gradient of W_{11}) causes $\hat{v}_{22} \ll \hat{v}_{11}$, so Adam's effective learning rate in the $(2,2)$ direction is $\approx 10\times$ larger. This over-updates W_{22}, potentially pushing $W_{2,:}^\top x$ below zero for all x.

Why ReDo fixes this: ReDo detects dead neurons and reinitialises their incoming and outgoing weights, breaking the feedback loop at step 3. The neuron re-enters the activation region, gradients resume, $\hat{v}$ grows, and the large-learning-rate problem dissolves.

4.15.3 Quantitative Analysis

At step T with dead fraction ϕ, the effective gradient has support on $(1-\phi)d$ neurons. The second moment for dead neurons satisfies $\hat{v}_{t,i}^{\text{dead}} = \varepsilon^2 \cdot \beta_2^t$ (pure decay). The effective learning rate for dead neurons is η/ε — a factor $1/\varepsilon = 10^8$ larger than intended.

The spurious update magnitude for a dead neuron over T steps is bounded by:

$$|\Delta W_i|_{\text{dead}} \leq \frac{\eta}{\varepsilon} \cdot T \cdot |\hat{m}_i|_{\max},$$

where $|\hat{m}_i|_{\max}$ is the maximum accumulated momentum (due to early-training gradients). For $T = 10^5$ steps, $\eta = 10^{-3}$, $\varepsilon = 10^{-8}$: $|\Delta W_i| \leq 10^5 \times 10^{-3}/10^{-8} \times |\hat{m}| = 10^{10} \times |\hat{m}|$. Even a tiny $|\hat{m}| = 10^{-12}$ (residual from early training) gives $|\Delta W_i| \leq 0.01$, which is enough to displace a near-zero weight and kill an already-marginal neuron.

This calculation makes Conjecture 4.31 plausible: the large effective learning rate for dead neurons ($\eta/\varepsilon \gg \eta$) can drive dead neurons further from the activation region, accelerating the dormancy spiral. What is missing for a proof is a rigorous bound on the direction of the spurious update (whether it systematically moves toward or away from the activation region).

4.16 The Complete Optimal Control Theory of Plasticity

Section 4.3 formulated plasticity preservation as an optimal control problem and derived the Pontryagin necessary conditions (Proposition 4.3.1). This section solves the control problem explicitly for tractable special cases and discusses approximation strategies for general networks.

4.16.1 The LQR Special Case

When the loss is quadratic ($L_t(w) = \frac{1}{2} w^\top H w - b^\top w$ for time-varying H_t, b_t) and the plasticity functional is quadratic ($\mathcal{P}(w) = w^\top P w$ for positive definite P), the optimal control problem (4.2) becomes a *Linear-Quadratic Regulator* (LQR).

Proposition 4.35 (LQR solution for plasticity control)**.** *For the quadratic special case with state equation $\dot{w} = -H_t w + b_t + u$, plasticity $\mathcal{P}(w) = w^\top P w / \|P\|_F$, and control cost $\|u\|^2$: the optimal control is a linear feedback law:*

$$u^*(t) = -K(t)(w(t) - w_{\text{ref}}(t)),$$

where $K(t) \in \mathbb{R}^{d \times d}$ is the time-varying feedback gain matrix satisfying the Riccati ODE:

$$\dot{K} = K H_t + H_t^\top K - K K/\kappa + \lambda^* P,$$

and $w_{\text{ref}}(t)$ is the reference trajectory (the unconstrained minimiser of L_t).

Proof. This follows directly from the Pontryagin Maximum Principle applied to the linear system with quadratic running cost $L_t(w) + \lambda^*(\mathcal{P}_{\min} - \mathcal{P}(w))$. The Hamiltonian is: $\mathcal{H}(w, p, u) = p^\top(-Hw + b + u) - \frac{1}{2}w^\top Hw + b^\top w - \lambda^*(w^\top Pw - P_{\min})$. The optimal control is $u^* = \kappa p^*$ (from the ℓ_2 control constraint at the boundary). The costate equation $\dot{p}^* = Hp^* + Hw - b + 2\lambda^* Pw$ is linear in (w, p), and the combined system has the Riccati structure. □

Example 4.36 (Explicit solution for $d = 1$)**.** For $d = 1$, $H = 1$, $P = 1$, $\lambda^* = 1$, $\kappa = 1$, $T = 10$: The Riccati equation is $\dot{k} = 2k - k^2 + 1$ with boundary condition $k(T) = 0$. This is a Bernoulli ODE, solvable explicitly: $k(t) = 1 + \sqrt{2}\coth(\sqrt{2}(T - t) + c)$ for some constant c. The optimal gain is $k(0) \approx 1 + \sqrt{2}\coth(\sqrt{2} \cdot 10) \approx 1 + \sqrt{2} \approx 2.41$.

The optimal control is $u^*(t) = -k(t)(w(t) - w^*)$, where $w^* = 1$ (the minimiser of $L = \frac{1}{2}(w - 1)^2$). This is a damping control: when w moves away from w^* (losing plasticity by moving to the boundary of the plasticity constraint), the control pushes it back, at cost proportional to the displacement from the optimal trajectory.

4.16.2 Approximate Dynamic Programming

For general non-quadratic losses and plasticity functionals, the exact optimal control is intractable. *Approximate dynamic programming* (ADP) approximates the value function $V(w, t) = \min_u \int_t^T L_s(w(s))\, ds$ subject to the system dynamics.

Definition 4.37 (Value function for plasticity control)**.** The value function $V : \mathbb{R}^d \times [0, T] \to \mathbb{R}$ for problem (4.2) satisfies the Hamilton–Jacobi–Bellman (HJB) equation:

$$-\frac{\partial V}{\partial t}(w, t) = \min_{\|u\| \le \kappa} \left[L_t(w) + \nabla_w V(w, t)^\top(-\nabla L_t(w) + u) + \lambda^*(p_{\min} - \mathcal{P}(w)) \right].$$

The minimum over u is attained at $u^* = \kappa \nabla_w V(w, t) / \|\nabla_w V(w, t)\|$ (bang-bang control), giving:

$$-\frac{\partial V}{\partial t} = L_t(w) - \nabla_w V^\top \nabla L_t + \kappa \|\nabla_w V\| + \lambda^*(p_{\min} - \mathcal{P}(w)).$$

The ADP approach approximates $V(w, t) \approx \hat{V}(w, t; \theta)$ using a neural network with parameters θ (a "critic" network), trained by minimising the Bellman residual:

$$\mathcal{L}_{\text{Bellman}}(\theta) = \mathbb{E}\left[\left(\hat{V}(w, t; \theta) - L_t(w)\Delta t - \hat{V}(w', t + \Delta t; \theta) \right)^2 \right],$$

where $w' = w + \Delta t(-\nabla L_t(w) + u^*)$ is the next state under the optimal control (estimated from $\hat{V}$). This is the deep reinforcement learning approach applied to the plasticity control problem.

Remark 4.38. The ADP approach to plasticity control is novel and undeveloped in the literature. It would require:

1. A critic network $\hat{V}$ trained online alongside the main network.
2. A plasticity functional $\mathcal{P}$ that is differentiable (using smooth approximations to the dead neuron indicator).
3. A control signal u^* derived from $\nabla_w \hat{V}$, applied as an additive correction to the gradient update.

This "plasticity-aware ADP" would be a principled algorithm that automatically adjusts its regularisation strength based on the current plasticity state — activating the control only when $\mathcal{P}(w) < p_{\min}$ (complementary slackness) and deactivating it when the network has recovered plasticity. This is significantly more adaptive than ReDo (which activates reinitialisation every Δ steps regardless of current plasticity) or Shrink-and-Perturb (which applies a fixed perturbation schedule).

4.17 The Wasserstein Gradient Flow: Complete Theory

Section 4.6 introduced the Wasserstein gradient flow formulation of continual learning. This section develops the theory completely, including the JKO scheme and the particle approximation.

4.17.1 The JKO Scheme: Wasserstein Gradient Flow as Proximal Steps

The Wasserstein gradient flow of $\mathcal{F}(\mu)$ can be discretised using the *Jordan–Kinderlehrer–Otto* (JKO) scheme:

Definition 4.39 (JKO scheme)**.** The JKO scheme for the Wasserstein gradient flow of $\mathcal{F}$ with time step τ is:

$$\mu_{t+1} = \arg\min_{\mu} \left[\mathcal{F}(\mu) + \frac{1}{2\tau} W_2^2(\mu, \mu_t) \right].$$

This is the *proximal point algorithm* in the Wasserstein space: each step minimises $\mathcal{F}$ while staying close to the previous distribution (in the W_2 metric).

Theorem 4.40 (JKO scheme converges to the gradient flow)**.** *As $\tau \to 0$, the JKO iterates μ_t converge to the Wasserstein gradient flow $(\mu_t)_{t\geq 0}$ satisfying $\partial_t \mu_t = \operatorname{div}(\mu_t \nabla_w \delta\mathcal{F}/\delta\mu)$.*

Proof sketch. The key step is showing that the JKO minimiser satisfies, to first order in τ: $\mu_{t+1}(w) \propto \mu_t(\phi^{-1}(w))|\det \nabla\phi^{-1}(w)|$, where $\phi(w) = w - \tau\nabla_w(\delta\mathcal{F}/\delta\mu)(w)$ is the optimal transport map from μ_t to μ_{t+1}. This is the Euler–Lagrange equation for the JKO minimisation. As $\tau \to 0$, $\phi(w) \approx \mathrm{Id} - \tau\nabla_w(\delta\mathcal{F}/\delta\mu)$, and the continuity equation $\partial_t\mu + \operatorname{div}(\mu v) = 0$ with $v = -\nabla_w(\delta\mathcal{F}/\delta\mu)$ gives the gradient flow. □

4.17.2 The JKO Scheme for Continual Learning

For the continual learning functional $\mathcal{F}_k(\mu) = \int L_k \, d\mu + \beta \, \mathrm{KL}(\mu\|\pi_{k-1})$: the JKO step is:

$$\mu_{\text{new}} = \arg\min_{\mu} \left[\int L_k \, d\mu + \beta \, \mathrm{KL}(\mu\|\pi_{k-1}) + \frac{1}{2\tau} W_2^2(\mu, \mu_{\text{old}}) \right].$$

This combines three objectives:

1. Minimise task k loss.
2. Stay close to the previous task's posterior π_{k-1} (forgetting resistance).
3. Stay close to the current distribution μ_{old} in Wasserstein distance (stability of learning).

Proposition 4.41 (JKO as EWC in the Gaussian approximation)**.** *When $\pi_{k-1} = \mathcal{N}(w^{(k-1)}, F^{(k-1)-1})$ (Gaussian Laplace approximation to the previous task posterior) and $\mu_{\text{old}} = \mathcal{N}(\hat{w}, \sigma^2 I)$ (current Gaussian approximation), the JKO step reduces to:*

$$w_{\text{new}} = \arg\min_{w} \left[L_k(w) + \frac{\beta}{2}(w - w^{(k-1)})^\top F^{(k-1)}(w - w^{(k-1)}) + \frac{1}{2\tau\sigma^2} \|w - \hat{w}\|^2 \right],$$

which is the EWC loss (equation (4.5)) plus a proximal term in w.

Proof. For Gaussian distributions, the KL divergence and W_2 distance have explicit forms: $\mathrm{KL}(\mathcal{N}(\mu,\Sigma)\|\mathcal{N}(\nu,\Lambda)) = \frac{1}{2}[(\mu-\nu)^\top\Lambda^{-1}(\mu-\nu) + \operatorname{tr}(\Lambda^{-1}\Sigma) - d + \log(\det\Lambda/\det\Sigma)]$. $W_2^2(\mathcal{N}(\mu_1,\Sigma_1),\mathcal{N}(\mu_2,\Sigma_2)) = \|\mu_1-\mu_2\|^2 + \operatorname{tr}(\Sigma_1+\Sigma_2-2(\Sigma_1^{1/2}\Sigma_2\Sigma_1^{1/2})^{1/2})$. For $\Sigma_1 = \Sigma_2 = \sigma^2 I$: $W_2^2 = \|\mu_1-\mu_2\|^2$. The JKO minimisation over Gaussian means w (fixing variance $\sigma^2 I$) gives the stated formula. □

4.17.3 Particle Methods and SVGD

The particle approximation of the Wasserstein gradient flow (Section 4.6.2) uses N particles $\{w^{(i)}\}_{i=1}^N$ to represent the distribution $\mu_t \approx \frac{1}{N}\sum_i \delta_{w^{(i)}}$. The particle flow equation is:

$$\dot{w}^{(i)} = -\nabla_{w^{(i)}} \frac{\delta \mathcal{F}}{\delta \mu}(w^{(i)}) = -\nabla L_k(w^{(i)}) - \beta \nabla_w \log \mu_t(w^{(i)}) + \beta \nabla_w \log \pi_{k-1}(w^{(i)}).$$

The term $\nabla_w \log \mu_t(w^{(i)})$ (the score of the particle distribution) is estimated using a kernel density estimator:

$$\nabla_w \log \mu_t(w^{(i)}) \approx \frac{\sum_j K(w^{(i)}, w^{(j)}) \nabla_{w^{(i)}} K(w^{(i)}, w^{(j)})}{\sum_j K(w^{(i)}, w^{(j)})},$$

where K is a kernel (e.g., RBF). Substituting gives the SVGD (Stein Variational Gradient Descent) update:

$$w_{t+1}^{(i)} = w_t^{(i)} - \eta \sum_{j=1}^{N} \left[K(w_t^{(j)}, w_t^{(i)}) \nabla_{w^{(j)}} L_k(w_t^{(j)}) + \nabla_{w^{(j)}} K(w_t^{(j)}, w_t^{(i)}) \right].$$

Remark 4.42 (SVGD for continual learning). SVGD applied to the continual learning functional gives a particle-based algorithm where each particle $w^{(i)}$ is a full copy of the model. The particles interact through the kernel K, which encourages diversity (the second term in the SVGD update pushes particles apart). This diversity prevents all particles from collapsing to the same minimum of L_k, maintaining the diversity needed to represent the posterior over tasks.

The computational cost is $O(N^2)$ per step (all pairwise interactions), making SVGD impractical for large N. In practice, $N = 3$–10 particles are used, giving a 3–10× computational overhead. This is the deep ensemble approach: multiple independent models with interaction.

4.18 Progressive Networks: Capacity and Transfer

Section 4.7 introduced progressive networks as a capacity-allocation approach to continual learning. We now develop the theory of transfer via lateral connections.

4.18.1 Transfer via Lateral Connections

In a progressive network (Definition 4.7.1), the lateral connections $U_l^{(k,j)}$ (from column j to column k at layer l) enable the new task k to reuse features from previous tasks $j < k$.

Definition 4.43 (Transfer efficiency)**.** The *transfer efficiency* of lateral connection $U_l^{(k,j)}$ is:

$$\tau_l^{(k,j)} = \frac{\left\| U_l^{(k,j)} h_{l-1}^{(j)} \right\|_2}{\left\| W_l^{(k)} h_{l-1}^{(k)} \right\|_2},$$

the ratio of the lateral contribution to the direct contribution to layer l of column k. High τ indicates that column k is heavily using features from column j.

Proposition 4.44 (Transfer and task similarity)**.** *If tasks $\mathcal{T}_j$ and $\mathcal{T}_k$ have similar optimal representations (i.e., the optimal features for $\mathcal{T}_j$ are useful for $\mathcal{T}_k$), then the learned lateral connections $U_l^{(k,j)}$ will have high transfer efficiency $\tau_l^{(k,j)}$, and the column k will need fewer free parameters to achieve good performance on $\mathcal{T}_k$.*

Proof sketch. If $h_{l-1}^{(j)}$ (features from column j) are good features for $\mathcal{T}_k$, then the gradient of L_k with respect to $U_l^{(k,j)}$ is large (the gradient signal flows through the lateral connection), causing $U_l^{(k,j)}$ to grow in norm. Meanwhile, $W_l^{(k)}$ receives a smaller gradient (less new information is needed beyond what column j provides), staying smaller. The ratio $\tau_l^{(k,j)}$ increases. □

4.18.2 PackNet: Optimal Mask Selection

The PackNet saliency score $|w_i| \cdot |\nabla_{w_i} L_k|$ (Section 4.7.1) is a heuristic for selecting the most important parameters for task k. We show it is the first-order approximation to the optimal mask.

Proposition 4.45 (PackNet as greedy constrained optimisation)**.** *The optimal binary mask $m \in \{0,1\}^d$ retaining exactly $r \cdot d$ parameters, maximising the expected loss decrease after one gradient step with the masked gradient, satisfies:*

$$m_i^* = \mathbf{1}\left[|w_i| \cdot |\nabla_{w_i} L_k| \geq \theta_{r \cdot d}\right],$$

where $\theta_{r \cdot d}$ is the $(1-r)$-quantile of the saliency scores $|w_i| \cdot |\nabla_{w_i} L_k|$. This is the greedy solution to the integer program:

$$\max_{m \in \{0,1\}^d, \sum_i m_i = r \cdot d} \sum_i m_i \cdot |w_i| \cdot |\nabla_{w_i} L_k|.$$

Proof. The expected loss decrease after one step with the masked gradient $g^m = m \odot \nabla L_k$ (zeroing out unmasked entries) is: $\Delta L \approx -\eta \langle \nabla L_k, g^m \rangle = -\eta \sum_i m_i (\nabla_{w_i} L_k)^2$. The Taylor expansion of $L_k(w - \eta m \odot \nabla L_k)$ to second order adds a positive curvature term: $+\frac{\eta^2}{2} \sum_i m_i \lambda_i (\nabla_{w_i} L_k)^2$. For small η, the first-order term dominates. Maximising $\sum_i m_i (\nabla_{w_i} L_k)^2$ over binary m with $\sum_i m_i = r \cdot d$ is equivalent to selecting the $r \cdot d$ largest $|\nabla_{w_i} L_k|^2$.

However, the PackNet heuristic uses $|w_i| \cdot |\nabla_{w_i} L_k|$ rather than $(\nabla_{w_i} L_k)^2$. This corresponds to the second-order approximation: for weights near convergence, $|\nabla_{w_i} L_k| \approx \lambda_i |w_i - w_i^*| \approx \lambda_i |w_i|$ (if $w_i^* \approx 0$, i.e., the task-specific minimum is near zero). So $|w_i| \cdot |\nabla_{w_i} L_k| \approx |w_i|^2 \lambda_i$, which is the curvature-weighted amplitude — the "importance" of each parameter in the loss landscape. □

4.19 Rates of Plasticity Loss: Empirical Laws and Theoretical Bounds

While the proof of a general plasticity decay rate is an open problem (Open Problem 4.10.2), we can derive bounds for specific models and optimisers.

4.19.1 Dead Neuron Accumulation Rate for SGD

Proposition 4.46 (Dead neuron accumulation bound for SGD)**.** *For a ReLU network trained with SGD (learning rate η, batch size B) on a stationary distribution, under mild assumptions on the data distribution:*

$$\mathbb{E}[\phi_{\text{dead}}^{(l)}(w_T)] \leq \phi_{\text{dead}}^{(l)}(w_0) + C\sqrt{\frac{\eta T}{B}} \cdot d_l^{-1/2},$$

where C depends on the Lipschitz constant of the loss and the data distribution.

Proof. Model each neuron's pre-activation $z_i = w_i^\top x + b_i$ as a one-dimensional process. Under SGD, $w_{t+1} = w_t - \eta \hat{g}_t$, so $z_i(w_{t+1}) = z_i(w_t) - \eta \hat{g}_t^\top x_i^*$ where x_i^* is the effective input to neuron

i. The pre-activation performs a random walk with step size $\eta \|\hat{g}\| \|x_i^*\| / (B^{1/2})$ and drift $-\eta \mathbb{E}[\hat{g}]^\top x_i^*$ (the signal).

A neuron becomes permanently dead when its pre-activation drifts below $-R$ (the radius of the data support), escaping the activation region. The probability of this event by time T is bounded by Azuma's inequality applied to the martingale $z_i(w_t) - \mathbb{E}[z_i(w_t)]$:

$$\mathbb{P}[z_i(w_T) \leq 0 \,|\, z_i(w_0) > 0] \leq \exp\left(-\frac{z_i(w_0)^2}{2\eta^2 T \|x_i^*\|^2 / B} \right).$$

Averaging over neurons with $z_i(w_0) > 0$ and the distribution of $z_i(w_0)$:

$$\mathbb{E}[\phi_{\text{dead}}(w_T) - \phi_{\text{dead}}(w_0)] \leq C\sqrt{\eta T / B},$$

where C depends on the density of neurons near the boundary $z_i \approx 0$. □

Remark 4.47. The bound $C\sqrt{\eta T/B}$ has the correct scaling:

- Larger η (larger step size): faster plasticity loss ($\propto \sqrt{\eta}$).
- Larger T (more training): more plasticity loss ($\propto \sqrt{T}$).
- Larger B (larger batch): slower plasticity loss ($\propto 1/\sqrt{B}$), because gradient noise is smaller, so the random walk is slower.

These predictions are qualitatively consistent with the empirical findings of Lyle et al. (2023), who observe that Adam (effectively larger η in sharp directions) causes faster plasticity loss than SGD, and larger batch sizes slow the loss.

4.19.2 Effective Rank Decay Rate

Proposition 4.48 (Effective rank decay under gradient descent)**.** *For a linear layer W_t trained by gradient descent on a task with gradient covariance $\Sigma_g = \mathbb{E}[\nabla_W L \nabla_W L^\top]$ of rank r ($r < \min(m, n)$):*

$$\frac{d}{dt}\text{rank}_{\text{eff}}(W_t) \leq -\eta \cdot \frac{r}{\min(m,n)} \cdot \text{rank}_{\text{eff}}(W_t),$$

giving exponential decay $\text{rank}_{\text{eff}}(W_t) \leq \text{rank}_{\text{eff}}(W_0) e^{-\eta r t / \min(m,n)}$.

Proof. The gradient of the loss with respect to W lies in the column space of Σ_g, which has rank r. Each gradient step moves W in a direction that is supported on at most r singular directions. By the von Neumann trace inequality, the effective rank of W_{t+1} is at most $r + \text{rank}_{\text{eff}}(W_t) \cdot (1 - \eta \lambda_{\min}^+(\Sigma_g))$. For $r \ll \min(m, n)$, the rank grows toward r and the remaining directions decay. The bound follows from a convexity argument on the Shannon entropy of the singular value distribution. □

Remark 4.49. This explains the empirical observation that Adam-trained networks show faster rank collapse: Adam's diagonal preconditioning effectively increases the learning rate in the dominant singular directions (those with large gradient second moments), accelerating the concentration of singular value mass in those directions and thus accelerating rank collapse. The effective learning rate in direction i is $\eta / \hat{v}_i^{1/2} \propto \eta / |\sigma_i|$ (for stationary training), which is larger for smaller singular values (flatter directions). This *amplifies* the rank collapse: the small singular directions get disproportionately large effective learning rates, causing them to be updated aggressively — but since these directions carry little gradient signal (they are in the null space of Σ_g), the updates are noisy and cause diffusion rather than descent, eventually pushing those singular values to zero.

4.20 Replica Theory and the Continual Learning Landscape

The statistical physics of spin glasses provides a framework for understanding the structure of the loss landscape in continual learning — specifically, how multiple task constraints interact in the parameter space.

4.20.1 The Gardner Phase Transition in Continual Learning

For a network with d parameters trained on K sequential tasks, each with n_k samples, the question "does a parameter vector exist that satisfies all task constraints simultaneously?" admits a sharp answer in terms of the total load $\alpha = \sum_k n_k/d$.

Theorem 4.50 (Gardner capacity for continual learning, informal)**.** *For a perceptron network (L layers, width d, K tasks with n samples each) trained with EWC regularisation:*

1. *For $\alpha = Kn/d < \alpha_c$ (below capacity): a parameter vector satisfying all task constraints simultaneously exists with high probability. The EWC solution $w^{(K)}$ achieves near-zero loss on all tasks.*

2. *For $\alpha > \alpha_c$ (above capacity): no single parameter vector can satisfy all constraints. The EWC solution has positive loss on at least one task, and the loss grows as $O((\alpha - \alpha_c)^{3/2})$ near the transition.*

The critical capacity α_c depends on the regularisation strength λ: $\alpha_c(\lambda) \approx \alpha_c(0) + C\lambda$ (regularisation increases capacity by keeping parameters near the origin, freeing space for new tasks).

Proof sketch via replica method. The Gardner volume (the volume of parameter space satisfying all task constraints) is: $V_K = \int \prod_{k=1}^{K} \prod_{i=1}^{n_k} \mathbf{1}[y_i^{(k)} f_w(x_i^{(k)}) \geq 1]\, d\mu(w)$, where $d\mu(w) = e^{-\lambda\|w\|^2/2} dw$ (Gaussian prior / EWC regularisation). The replica method computes $\mathbb{E}[\log V_K]$ by evaluating $\mathbb{E}[V_K^n]$ for integer n and analytically continuing to $n \to 0$. The saddle-point equations of the replica calculation give the critical load α_c as the solution to: $\alpha_c = \int_0^\infty (t + h)^2 \mathcal{D}t \cdot$ (order parameter equation), where the integral is over a Gaussian measure $\mathcal{D}t$ and h is the replica-symmetric order parameter (the self-consistency equation). At $\lambda = 0$, this gives $\alpha_c \approx 2$ (the Vapnik covering number bound for perceptrons); for $\lambda > 0$, α_c increases. □

Remark 4.51 (Practical implications). The Gardner capacity theorem gives a sharp prediction for when continual learning "works": for K tasks with n samples each and d parameters, the algorithm can succeed only when $Kn < \alpha_c d$. For a transformer with $d = 10^9$ parameters and $K = 100$ tasks with $n = 10^6$ samples each: $Kn/d = 100 \times 10^6/10^9 = 0.1$, well below $\alpha_c \approx 2$. This explains why large models can handle continual learning more easily: their large d increases the effective capacity.

The phase transition at α_c also explains the "catastrophic forgetting cliff": as the number of tasks increases, the algorithm works well below α_c, then fails abruptly above it (the loss on old tasks diverges). This is qualitatively consistent with the empirical observation that catastrophic forgetting gets worse suddenly when task count exceeds a threshold.

4.20.2 Overlap Matrix and Task Interference

The replica calculation introduces the *overlap matrix* $Q_{kk'} = \frac{1}{d}\left\langle w^{(k)}, w^{(k')} \right\rangle$ (normalised inner product between the parameters after tasks k and k').

Definition 4.52 (Task interference via overlap)**.** Tasks $\mathcal{T}_k$ and $\mathcal{T}_{k'}$ *interfere* if $Q_{kk'} < 0$: the parameter vectors optimal for each task point in opposite directions. They *reinforce* if $Q_{kk'} > 0$: the optimal parameter vectors are aligned.

The EWC penalty effectively constrains $Q_{kk'} \approx Q_{kk}$ (keeping the new parameter vector close to the old one). The GPM null-space projection constrains $Q_{kk'} = 0$ in the gradient directions (orthogonal updates). Progressive networks allow $Q_{kk'} = 0$ by construction (separate columns).

In the replica symmetric (RS) approximation, the order parameter $Q_{kk'} = q$ (same for all pairs) for well-separated tasks ($k \neq k'$), and $Q_{kk} = 1$ (unit norm normalisation). The RS solution is stable when $\lambda\alpha < 1$ (low task load); it breaks down (RSB) when $\lambda\alpha > 1$, signalling the onset of catastrophic forgetting.

4.21 Complete Analysis: EWC on Multi-Task Gaussian Problems

We develop a complete analytical treatment of EWC for Gaussian tasks, where all quantities are exactly computable.

4.21.1 The Multi-Task Gaussian Setting

Definition 4.53 (Gaussian task sequence)**.** A *Gaussian task sequence* consists of K tasks $\mathcal{T}_k$ with:

- Task loss: $L_k(w) = \frac{1}{2}(w - \mu_k)^\top \Lambda_k (w - \mu_k)$ (quadratic, centred at μ_k).
- Fisher matrix: $F^{(k)} = \Lambda_k$ (exact, since the Hessian equals the Fisher for Gaussian models).
- True optimal weights: $\mu_k \in \mathbb{R}^d$ (the task-specific minimum).

Proposition 4.54 (EWC on Gaussian tasks: closed-form solution)**.** *For a Gaussian task sequence with EWC regularisation strength λ: the EWC solution after K tasks satisfies the recursion:*

$$w^{(K)} = \Sigma_K \sum_{k=1}^{K} \lambda \Lambda_k \mu_k, \qquad \Sigma_K^{-1} = \lambda \sum_{k=1}^{K} \Lambda_k,$$

i.e., $w^{(K)}$ is the Λ_k-weighted average of the task means μ_k.

Proof. By induction. After task 1: $w^{(1)} = \mu_1$ (direct minimisation of L_1). After task 2 with EWC: minimise $L_2(w) + \frac{\lambda}{2}(w - w^{(1)})^\top F^{(1)}(w - w^{(1)}) = \frac{1}{2}(w - \mu_2)^\top \Lambda_2 (w - \mu_2) + \frac{\lambda}{2}(w - \mu_1)^\top \Lambda_1 (w - \mu_1)$. Setting the gradient to zero: $\Lambda_2(w - \mu_2) + \lambda\Lambda_1(w - \mu_1) = 0$, giving $(\Lambda_2 + \lambda\Lambda_1)w = \Lambda_2\mu_2 + \lambda\Lambda_1\mu_1$. So $w^{(2)} = (\Lambda_2 + \lambda\Lambda_1)^{-1}(\Lambda_2\mu_2 + \lambda\Lambda_1\mu_1)$.

After task K: by induction, the accumulated EWC penalty is $\frac{\lambda}{2}\sum_{k=1}^{K-1}(w - w^{(k-1)})^\top \Lambda_k (w - w^{(k-1)})$, which (after simplification via completing the square) reduces to $\frac{\lambda}{2}(w - \bar{\mu}_{K-1})^\top (\lambda \sum_{k=1}^{K-1} \Lambda_k)(w - \bar{\mu}_{K-1}) + \text{const}$, where $\bar{\mu}_{K-1}$ is the weighted mean. Minimising $L_K + \lambda \times$penalty gives the stated formula. □

Example 4.55 (EWC on isotropic Gaussian tasks)**.** For isotropic tasks: $\Lambda_k = I$ (identity), K tasks with means μ_k at the vertices of a regular simplex in $\mathbb{R}^d$ (maximally spread): $\langle \mu_k, \mu_{k'} \rangle = -1/(K-1)$ for $k \neq k'$, $\|\mu_k\|^2 = 1$.

EWC solution: $w^{(K)} = (\lambda K I)^{-1}(\lambda \sum_k \mu_k) = \frac{1}{K}\sum_k \mu_k = \bar{\mu}$. For the regular simplex: $\bar{\mu} = 0$ (the centroid of a regular simplex is the origin). So $w^{(K)} = 0$ regardless of λ!

This shows that for maximally interfering tasks (regular simplex means), EWC collapses to the origin — the worst possible solution (zero prediction for all tasks). The loss on task k at $w = 0$: $L_k(0) = \frac{1}{2}\|\mu_k\|^2 = \frac{1}{2}$.

Contrast with fine-tuning: $w_{\text{FT}}^{(K)} = \mu_K$ (only remembers last task). Loss on task k: $L_k(\mu_K) = \frac{1}{2}\|\mu_K - \mu_k\|^2 = 1$ for $k \neq K$ (complete forgetting). Loss on task K: $L_K(\mu_K) = 0$.

The EWC–fine-tuning trade-off on this example:

Algorithm	L_k for $k < K$	L_K	Sum $\sum_k L_k$
Fine-tuning	1.0	0.0	$K-1$
EWC ($\lambda > 0$)	0.5	0.5	$K/2$
Progressive networks	0.0	0.0	0
Optimal joint	$(K-1)/(K(K-1)) = 1/K$	$1/K$	1

Table 4.4: Loss comparison for isotropic tasks on a regular simplex.

EWC achieves sum loss $K/2$ vs. fine-tuning's $K-1$ and optimal joint training's 1. EWC is better than fine-tuning by factor ≈ 2, but far from optimal because the tasks are maximally interfering (the optimal joint solution averages to the origin but uses the Fisher weighting to partially recover the task means).

Example 4.56 (EWC on aligned tasks)**.** For tasks with aligned means: $\mu_k = k \cdot e_1$ (all in the same direction e_1), $\Lambda_k = I$: $w^{(K)} = \frac{1}{\lambda K}\lambda \sum_k k e_1 = \frac{K(K+1)}{2K} e_1 = \frac{K+1}{2} e_1$. Loss on task k: $L_k(w^{(K)}) = \frac{1}{2}(\frac{K+1}{2} - k)^2$.

The EWC solution places the weights at the centroid $\bar{\mu} = \frac{K+1}{2} e_1$, which is the optimal for the average loss $\frac{1}{K}\sum_k L_k$ (since the Hessians are isotropic). For aligned tasks, EWC is *exactly optimal*. This is the case where continual learning is easiest: all tasks point in the same direction, so there is no trade-off.

4.22 Complete Solution to Chapter 4 Exercises

Exercise 4.6 (Complete solution)**. Exercise 4.2**: Prove Proposition 4.6.1 for two quadratic tasks.

$L_1(w) = \frac{1}{2}\|w - a\|^2$, $L_2(w) = \frac{1}{2}\|w - b\|^2$ with $a \neq b$.

Step 1: Gibbs posterior after task 1 (temperature T): $\pi_1(w) \propto e^{-L_1(w)/T} = e^{-\|w-a\|^2/(2T)} = \mathcal{N}(a, TI)$.

Step 2: Wasserstein gradient flow of $\mathcal{F}_2(\mu) = \int L_2 d\mu + \beta\,\mathrm{KL}(\mu\|\pi_1)$. First variation: $\frac{\delta \mathcal{F}_2}{\delta \mu}(w) = L_2(w) + \beta \log \frac{\mu(w)}{\pi_1(w)}$. Gradient: $\nabla_w \frac{\delta \mathcal{F}_2}{\delta \mu} = \nabla L_2(w) + \beta \nabla_w \log \mu(w) - \beta \nabla_w \log \pi_1(w) = (w - b) + \beta \nabla_w \log \mu - \frac{\beta}{T}(w - a)$.

Step 3: In the Gaussian ansatz $\mu_t = \mathcal{N}(m_t, \sigma_t^2 I)$: $\nabla_w \log \mu_t(w) = -(w - m_t)/\sigma_t^2$. $\nabla_w \log \pi_1(w) = -(w - a)/T$. The particle ODE: $\dot{w} = -(w - b) - \beta(-(w - m_t)/\sigma_t^2) + \beta(-(w - a)/T)$. For the mean: $\dot{m}_t = -(m_t - b) + 0 - \frac{\beta}{T}(m_t - a) = -(1 + \frac{\beta}{T})m_t + b + \frac{\beta a}{T}$.

Step 4: Fixed point $m_\infty = (b + \frac{\beta}{T}a)/(1 + \frac{\beta}{T}) = \frac{Tb + \beta a}{T + \beta}$. For $\beta \to \infty$: $m_\infty \to a$ (remember task 1). For $\beta \to 0$: $m_\infty \to b$ (learn task 2, forget task 1). ✓

Connection to EWC: The EWC solution with $\lambda = \beta/T$ and $F^{(1)} = I/T$: $w_{\text{EWC}}^* = (I + \lambda I)^{-1}(b + \lambda a) = (b + \lambda a)/(1 + \lambda) = m_\infty$ with $\lambda = \beta/T$. Identical!

Exercise 4.7 (Complete solution)**. Exercise 4.3**: Gradient conflict at $w = (0, 0, 0)$ for the GEM example.

Tasks: $L_k(w) = \frac{1}{2}\|w - e_k\|^2$ with $e_1 = (1, 0, 0)$, $e_2 = (0, 1, 0)$, $e_3 = (0, 0, 1)$. At $w_{\text{EWC}}^{(2)} = (1/2, 1/2, 0)$ (after task 2 with $\lambda = 1$):

$\nabla L_1(w^{(2)}) = w^{(2)} - e_1 = (-1/2, 1/2, 0)$. $\nabla L_2(w^{(2)}) = w^{(2)} - e_2 = (1/2, -1/2, 0)$. $\nabla L_3(w^{(2)}) = w^{(2)} - e_3 = (1/2, 1/2, -1)$.

Conflict check: $\langle \nabla L_3, \nabla L_1 \rangle = (1/2)(-1/2) + (1/2)(1/2) + (-1)(0) = 0$ (no conflict). $\langle \nabla L_3, \nabla L_2 \rangle = (1/2)(1/2) + (1/2)(-1/2) + (-1)(0) = 0$ (no conflict).

GEM projection: since $g_3 = (1/2, 1/2, -1)$ already satisfies $\langle g_3, g_1 \rangle \geq 0$ and $\langle g_3, g_2 \rangle \geq 0$, the GEM projection is $\tilde{g}_3 = g_3$ (no modification needed).

GEM update from $w^{(2)} = (1/2, 1/2, 0)$: gradient descent on L_3 with GEM constraint: $w^{(3)} \to e_3 = (0, 0, 1)$.

Final losses: $L_1(e_3) = \|(0,0,1) - (1,0,0)\|^2/2 = (1+1)/2 = 1$ (task 1 forgotten). $L_2(e_3) = \|(0,0,1) - (0,1,0)\|^2/2 = 1$ (task 2 forgotten). $L_3(e_3) = 0$ (task 3 learned perfectly).

This confirms the analysis of Section 4.5.2: GEM's first-order guarantee (inner product ≥ 0) does not prevent forgetting globally.

Exercise 4.8 (Complete solution)**. Exercise 4.5**: Verify that the Wasserstein gradient flow of $\mathcal{F}(\mu) = \int L(w)\, d\mu(w)$ reduces to the Fokker–Planck equation.

The first variation of $\mathcal{F}$ with respect to μ is: $\frac{\delta \mathcal{F}}{\delta \mu}(w) = L(w)$ (the functional derivative of a linear functional is just the integrand).

The Wasserstein gradient flow is (Definition 4.6.2): $\partial_t \mu_t = \operatorname{div}(\mu_t \nabla_w \frac{\delta \mathcal{F}}{\delta \mu}(\mu_t)) = \operatorname{div}(\mu_t \nabla_w L(w))$.

This is the Fokker–Planck equation for the deterministic flow $\dot{w} = -\nabla L(w)$: the probability density μ_t of the particle position w_t evolves according to $\partial_t \mu_t + \operatorname{div}(\mu_t(-\nabla L)) = 0$, which is equivalent to $\partial_t \mu_t = \operatorname{div}(\mu_t \nabla L)$. ✓ □

Chapter 5

Connecting Themes: A Unified Theory of Optimisation Geometry

The map is not the territory. But a good map of the territory — one that shows the mountains, the valleys, and the paths between them — is indispensable for the journey.

Chapter 5 is a synthesis chapter, designed to be a standalone reference. It can be read independently after the four preceding chapters, or used as a condensed overview before reading them in detail. Cross-references point to the detailed treatments.

5.1 Overview: Four Themes, One Geometry

The four preceding chapters address four apparently distinct problems: escape from saddle points (Chapter 1), the design of adaptive optimisers (Chapter 2), sharpness-aware minimisation (Chapter 3), and the long-horizon failure of plasticity (Chapter 4). This chapter argues that all four are facets of a single underlying structure: the *geometry of the loss landscape as encoded by its Hessian.*

The Hessian $H = \nabla^2 L(w)$ appears in every chapter:

- **Chapter 1**: The index of a critical point is the number of negative eigenvalues of H. The loss–index correlation (Corollary 1.3.1) is a statement about the expected spectral distribution of H at critical points of a random field.

- **Chapter 2**: Adam's second moment estimate $v_{t,i} \approx F_{ii}(w) \approx H_{ii}(w)$ (diagonal Fisher approximation). The edge of stability is determined by $\lambda_{\max}(H)$ relative to $2/\eta$ (or $2\hat{v}^{1/2}/\eta$ for Adam).

- **Chapter 3**: The sharpness in the PAC-Bayes bound is $\mathrm{tr}(H)$ (isotropic perturbation) or $\lambda_{\max}(H)$ (worst-case perturbation). SAM explicitly minimises the worst-case perturbation loss, which is controlled by $\lambda_{\max}(H)$.

- **Chapter 4**: The Fisher information matrix used in EWC is the curvature of the log-posterior — exactly the Hessian of the negative log-likelihood at the MAP estimate. The rank collapse measured by $\mathrm{rank}_{\mathrm{eff}}(W)$ corresponds to the low-rank structure of H (bulk + outliers, Proposition 1.7 and Section 1.3.3).

Key Result

Unifying principle. The Hessian $H = \nabla^2 L(w)$ is not merely a technical device but the fundamental geometric structure of the loss landscape. Understanding its spectral properties — its eigenvalue distribution, its low-rank structure, its evolution during training — is the key to principled optimiser design across all four domains.

5.2 The Unified Map: Flat Minima, Generalisation, Plasticity, and Saddle Escape

The conceptual map described below traces the connections between the four themes.

5.2.1 Node 1: Loss Landscape Geometry

The loss landscape is characterised by:

(a) The distribution of critical points: minima, saddle points, maxima. In high dimension, this is governed by the Åufinger–Ben Arous–Černý theorem (Theorem 1.3.1): high-index saddles are exponentially suppressed at low energy.

(b) The Hessian spectral structure at a trained minimum: bulk (Marchenko–Pastur) plus outliers (top r eigenvalues), as characterised in Section 1.7.

(c) The *sharpness* $\lambda_{\max}(H)$ and *trace* $\mathrm{tr}(H)$: two measures of how curved the minimum is.

5.2.2 Node 2: Saddle Escape and Training Efficiency

Saddle escape (Chapter 1) determines *how long* training takes to find a good minimum. The connections to other nodes:

- → **Adaptive optimisers**: Adam's per-coordinate step sizes modulate the escape rate in different directions. In directions with large $|\nabla L|$ (and thus large $\hat{v}$), Adam reduces the effective learning rate, which *slows* saddle escape in those directions. In directions with small $|\nabla L|$ (near a saddle's unstable direction), Adam increases the effective rate, which *accelerates* escape. The net effect is direction-dependent and architecture-specific.

- → **Sharpness**: gradient descent escapes saddle points and descends into a basin. The basin it finds is characterised by its sharpness $\lambda_{\max}(H)$. SGD with small batch size escapes saddle points more aggressively and settles in *flatter* basins (Proposition 1.5.2: larger noise → faster saddle escape → harder to re-enter sharp regions). This is the implicit regularisation argument for small-batch generalisation.

- → **Plasticity**: the time spent near saddle points during early training correlates with the development of dead neurons (the gradient signal is small near saddle points, causing some directions to become inactive). Fast saddle escape via SGD noise preserves more plastic configurations.

5.2.3 Node 3: Adaptive Optimisers and the Implicit Bias

Adam's behaviour (Chapter 2) connects to every other node:

- → **Saddle escape**: as above (direction-dependent modulation).

- → **Flat minima**: Adam finds different minima than SGD due to its ℓ^∞ implicit bias (Proposition 2.5.1). It does not systematically favour flat minima (it may find sharper ones in some settings). The edge of stability (Theorem 2.6.1) shows that Adam operates at a *higher* effective sharpness threshold than SGD, allowing training near sharper regions.

- → **Plasticity**: Adam's rank reduction (implicit ℓ^1-Schatten bias, Theorem 2.5.1) causes gradual effective rank collapse of weight matrices. Combined with ReLU dead neurons, this is the mechanism behind the dormancy spiral (Conjecture 4.9.1).

- → **EWC**: Adam's second moment $v_{t,i}$ approximates the diagonal Fisher $F_{ii}(w)$ (Proposition 2.8.1), directly providing the EWC importance weights for free (Section 4.4.2).

5.2.4 Node 4: Sharpness-Aware Minimisation

SAM (Chapter 3) explicitly targets flat minima. Its connections:

- → **Loss landscape**: SAM's minimax objective $\min_w \max_{\|\varepsilon\|\leq\rho} L(w+\varepsilon)$ directly selects for flat regions of the loss landscape. The PAC-Bayes bound (Theorem 3.5.1) provides the theoretical justification.

- → **Adam**: the edge of stability (Corollary 2.6.1) is an implicit sharpness control mechanism. SAM is an explicit one. When combined (AdamSAM), both mechanisms operate simultaneously — their interaction is theoretically unexplored (Open Problem 3.8.3).

- → **Plasticity**: flat minima have lower $\lambda_{\max}(H)$, meaning the loss is more uniformly curved. This suggests that wider basins are *more compatible* with plasticity (the network is not committed to a sharp feature direction). The sharpness–plasticity trade-off (Section 5.3) makes this precise.

5.2.5 Node 5: Plasticity and Continual Learning

Plasticity (Chapter 4) is the long-horizon manifestation of all the preceding phenomena:

- ← **Saddle escape**: fast saddle escape in early training preserves more live neurons and higher effective rank.

- ← **Adam implicit bias**: rank collapse is induced by Adam's second moment concentration (Conjecture 4.9.1).

- ← **Flat minima**: networks in flat minima are more robust to parameter perturbation, suggesting that flat minima are more plastic. This is the sharpness-plasticity trade-off — the key tension explored in the next section.

- → **EWC and continual learning**: the geometry of the loss landscape at a trained minimum (Hessian, Fisher) determines the EWC importance weights and hence the forgetting resistance.

5.3 The Sharpness–Plasticity Trade-Off

The most striking connection between Chapter 3 (SAM) and Chapter 4 (plasticity) is the apparent tension between flat minima and plasticity.

5.3.1 Flat Minima Generalise Better

By the PAC-Bayes bound (Theorem 3.5.1), flat minima (small $\lambda_{\max}(H)$) generalise better: the perturbation term $\max_{\|\varepsilon\|\leq\rho}[L(w+\varepsilon)-L(w)]$ is small. SAM explicitly seeks such minima.

5.3.2 Flat Minima May Impair Rapid Adaptation

Consider a network at a flat minimum w^* of task $\mathcal{T}_1$. When a new task $\mathcal{T}_2$ arrives, the gradient descent update is:

$$w_{t+1} = w_t - \eta \nabla L_2(w_t).$$

If w^* is flat (small $\lambda_{\max}(H_1)$), then w^* is in a wide basin of L_1. This is *good* for forgetting resistance: gradient descent on L_2 starting from w^* must travel further before L_1 increases significantly.

However, flatness of L_1 at w^* does not imply that w^* is a good initialisation for L_2. If $\nabla L_2(w^*) = 0$ (a saddle point of L_2), the network is trapped. More generally, the *plasticity* of the network — its ability to adapt quickly — depends not on the flatness of the current minimum but on the network's representational capacity (effective rank, live neurons), which may be independent of sharpness.

Proposition 5.1 (Sharpness and plasticity are not directly opposed)**.** *Let w^* be a flat minimum of L_1 (small $\lambda_{\max}(\nabla^2 L_1(w^*))$) and let $\mathcal{P}(w^*)$ be the plasticity functional (equation (4.1)). These two quantities are not monotonically related:*

1. *A network can be* flat and plastic*: wide basin, high effective rank, many live neurons. Example: early in training, before rank collapse.*
2. *A network can be* sharp and plastic*: narrow basin, high effective rank. Example: a freshly initialised network with random weights (high rank, somewhat sharp).*
3. *A network can be* flat and rigid*: wide basin but collapsed rank (few active singular directions). Example: a network after long Adam training, where rank collapse has occurred but the remaining singular directions are well-optimised.*
4. *A network can be* sharp and rigid*: the worst case for continual learning. Example: a network at the end of long fine-tuning on a narrow task.*

Proof. We provide explicit constructions for each case.

Case 1 (flat and plastic): Let $L_1(w) = \frac{\varepsilon}{2}\|w\|^2$ for small $\varepsilon > 0$. The minimum is $w^* = 0$ with $\lambda_{\max}(H_1) = \varepsilon$ (flat). Initialising with a random Gaussian weight matrix $W^{(l)} \in \mathbb{R}^{d\times d}$, the effective rank is $\mathrm{rank}_{\mathrm{eff}}(W^{(l)}) \approx d$ and no neurons are dead (randomly initialised ReLU networks have about 50% live neurons at each layer). So $\mathcal{P}(w^*) \approx 0.5 \times 2 = 1$.

Case 3 (flat and rigid): After long Adam training on a flat loss (e.g., continual regression with cosine similarity objective), the effective rank collapses to $O(\sqrt{d})$ via the dormancy spiral (Conjecture 4.31), but the remaining singular directions are well-aligned with the data, keeping the loss flat. $\lambda_{\max}(H_1) \approx \varepsilon$ but $\mathrm{rank}_{\mathrm{eff}}(W^{(l)}) \approx \sqrt{d} \ll d$.

Cases 2 and 4 follow analogously by appropriate construction of the loss. □

5.3.3 The Quantitative Trade-Off

Definition 5.2 (Sharpness-adjusted plasticity)**.** For a network at w^* with sharpness $\ell^* = \lambda_{\max}(\nabla^2 L(w^*))$ and plasticity $\mathcal{P}^* = \mathcal{P}(w^*)$, define the *sharpness-adjusted plasticity*:

$$\Pi(w^*) = \mathcal{P}^* \cdot \frac{1}{1+\alpha\ell^*},$$

where $\alpha > 0$ is a task-switch rate parameter.

The intuition: a flat minimum ($\ell^* \approx 0$) has $\Pi \approx \mathcal{P}^*$ (plasticity is not penalised by sharpness), while a sharp minimum ($\ell^* \gg 1/\alpha$) has $\Pi \approx \mathcal{P}^*/(\alpha\ell^*) \to 0$ (sharpness reduces effective plasticity).

The optimal algorithm for continual learning maximises $\Pi(w^*)$ simultaneously with minimising the training loss. This is the combination of SAM (for flatness) and ReDo (for plasticity):

1. SAM ensures ℓ^* is small (flat minimum, good generalisation).

2. ReDo ensures $\mathcal{P}^*$ is large (live neurons, high rank, good adaptability).

3. Together, they maximise $\Pi(w^*)$.

This combination has not been rigorously studied in the continual learning literature and represents a direct open problem.

5.4 The Implicit-Explicit Regularisation Duality

Every algorithm in this volume has both an implicit bias (what it does naturally, without explicit penalty) and can be modified with explicit regularisation (an added term to the loss).

Algorithm	Implicit bias	Explicit version
SGD	ℓ_2-min-norm solutions; flat minima via small batch	L2 regularisation ($+\lambda \|w\|^2$)
Adam	ℓ^∞-sparse solutions; low effective rank	AdamW (decoupled weight decay)
SGD on SAM loss	Flat minima (PAC-Bayes motivated)	ASAM (adaptive perturbation)
EWC	Near-previous-task solutions weighted by Fisher	Progressive networks (hard constraint)
ReDo	High plasticity near dead-neuron boundaries	DASH (gradient projected to plasticity boundary)

Table 5.1: Implicit versus explicit regularisation for the algorithms in this volume.

Remark 5.3. A recurring pattern: explicit regularisation is more controllable but more expensive; implicit regularisation is free but hard to tune. The research programme of understanding implicit biases is precisely the programme of converting "what the algorithm does" into "what the algorithm optimises" — giving practitioners the ability to target specific properties (flatness, sparsity, plasticity) by choosing the right algorithm rather than by adding cost to the loss.

5.5 Stationary vs. Non-Stationary: The Fundamental Divide

Chapters 1–3 assume a fixed, stationary loss function. Chapter 4 breaks this assumption. The transition is not merely a technical complication: it reveals qualitatively new phenomena.

Setting	Primary failure mode	Primary tool
Stationary, early training	Saddle point trapping	Perturbed GD, SGD noise (Ch. 1)
Stationary, convergent	Ill-conditioning, slow convergence	Adam, AdamW (Ch. 2)
Stationary, generalisation	Sharp minima, overfitting	SAM, SWA (Ch. 3)
Non-stationary, task switch	Catastrophic forgetting	EWC, GEM, GPM (Ch. 4)
Non-stationary, long horizon	Loss of plasticity	ReDo, Shrink-and-Perturb (Ch. 4)

Table 5.2: Failure modes and tools by training setting.

The key insight: the tools that succeed in the stationary setting (Adam for convergence, SAM for generalisation) may *cause* or *exacerbate* the non-stationary failure modes. Specifically:

- **Adam** causes faster rank collapse and dormancy (Conjecture 4.9.1) than SGD.
- **SAM** seeks flat minima, which resist forgetting — but the flat minimum may itself have lower plasticity if reached via Adam's implicit bias (Case 3 of Proposition 5.1).

This non-trivial interaction between optimiser design and long-horizon behaviour is the frontier of the field.

5.6 Open Conjectures and the Research Programme for Part IV

5.6.1 Open Conjectures

We collect the open problems from all four chapters and articulate the five most important.

Conjecture A: Adam-induced dormancy spiral (Conjecture 4.9.1)

Under mild conditions on the data distribution and architecture, the positive feedback loop between rank collapse and dead neuron growth under Adam is self-sustaining and irreversible without active intervention (reinitialisation or regularisation). Status: empirically supported, unproved.

Conjecture B: Anisotropic loss–index correlation

The loss–index monotonicity of Corollary 1.3.1 (proved for isotropic Gaussian fields) holds for the anisotropic fields with low-rank-plus-bulk Hessian structure observed in real neural networks. Status: partial results in the physics literature, no complete proof.

Conjecture C: SAM finds flatter minima than Adam without SAM

For Transformer training with a large number of steps, the sharpness $\lambda_{\max}(\nabla^2 L(w^*_{\text{SAM}})) < \lambda_{\max}(\nabla^2 L(w^*_{\text{Adam}}))$ with high probability, and the improvement translates to better population loss. Status: empirically observed, but the theoretical mechanism (PAC-Bayes bound implies better generalisation for SAM) is proved only in the bounded loss, PAC-Bayes framework — not for the specific loss functions used in LLM training.

Conjecture D: Optimal continual learning requires both flatness and plasticity

The optimal continual learning algorithm (maximising $\Pi(w^*)$ as defined in Section 5.3) is a combination of SAM (for flatness) and a plasticity-restoring mechanism (for rank and live neurons). No single existing algorithm achieves both simultaneously. Status: open; formalising Π and proving that existing algorithms are suboptimal is a concrete research direction.

Conjecture E: Schedule-Free Adam converges at the same rate as Adam with optimal schedule

Theorem 2.9.1 gives a convergence rate for Adam with decreasing step size $\eta_t = \eta/\sqrt{t}$. Schedule-Free Adam (Definition 2.7.1) achieves the same $O(T^{-1/4})$ rate without knowing the horizon T, via the online-to-batch conversion guarantee. Status: the online-to-batch guarantee is proved (Cesa-Bianchi et al., 2004), but whether it gives a matching $O(T^{-1/4})$ rate for Adam specifically (rather than the generic online learner) requires a more careful analysis.

5.6.2 The Research Programme for Part IV

Part IV of the Mathematics of Deep Learning series will address the statistical physics of learning dynamics: the connection between the microscopic training algorithm and the macroscopic behaviour of the loss and the learned representations. The open conjectures above suggest four specific directions:

1. **Random matrix theory for the Hessian at trained minima.** The bulk-outlier decomposition (Proposition 1.7.1) is observational. A rigorous RMT analysis would give the exact distribution of Hessian eigenvalues at convergence as a function of architecture, data distribution, and optimiser — enabling precise predictions of sharpness, generalisation gap, and plasticity.

2. **Dynamical systems theory for optimiser trajectories.** Adam, SAM, and their combinations are dynamical systems in the parameter space $\mathbb{R}^d$. The edge of stability (Section 2.6) shows that these systems have non-trivial attractors. A complete characterisation of the attractor geometry — where does the trajectory converge, and what determines the basin of attraction — would resolve Conjectures C and D.

3. **Information geometry of continual learning.** EWC, GEM, and the Wasserstein formulation all use different geometric structures (Fisher metric, Euclidean cone, Wasserstein distance) to define what it means to "stay close" to the previous task. A unified information-geometric framework would identify the optimal geometry for each setting and give a principled derivation of all known algorithms as special cases.

4. **Finite-width effects and the mean-field limit.** The Wasserstein gradient flow of Section 4.6 is a mean-field ($N \to \infty$) result. For practical single-model ($N = 1$) training, the finite-width corrections are the dominant effects. Quantifying these corrections — the finite-N analogue of the $1/\sqrt{N}$ CLT corrections — is essential for connecting theory to practice.

5.7 A Unified View: The Geometry of Learning Algorithms as Dynamical Systems

We close with the most general perspective: a learning algorithm is a dynamical system on a high-dimensional manifold, and understanding deep learning is understanding the interaction between the geometry of the manifold (determined by the architecture and the data) and the dynamics of the algorithm (determined by the optimiser and the schedule).

Definition 5.4 (Loss landscape manifold)**.** The *loss landscape manifold* is the Riemannian manifold (M, g_H) where M is the parameter space $\mathbb{R}^d$ (or a constrained submanifold with layer normalisation) and g_H is the metric induced by the Hessian $H = \nabla^2 L(w)$:

$$g_H(u, v) = u^\top H v \quad \text{(at a positive definite point)}.$$

In this metric, natural gradient descent (Definition 2.8.2) is the steepest descent direction, and the curvature tensor encodes the geometry of the loss landscape.

Definition 5.5 (Optimiser as flow on the manifold)**.** An optimiser defines a flow $\phi_t : M \to M$ (the map sending initial parameters to parameters after t gradient steps). The *invariant set* of the flow is the set of fixed points and limit cycles:

$$\mathrm{Inv}(\phi) = \{w : \phi_t(w) = w \ \forall t\} \cup \{\text{limit cycles of } \phi\}.$$

The results of this volume can be read as theorems about the invariant sets of different optimiser flows:

- **Chapter 1**: For SGD with noise, all saddle points are excluded from $\mathrm{Inv}(\phi_{\mathrm{PGD}})$ (strict saddles are escaped in polynomial time).
- **Chapter 2**: For Adam, the edge-of-stability attractor is a periodic orbit (or slow oscillation) near $\lambda_{\max}(H) \approx 2\hat{v}^{1/2}/\eta$.
- **Chapter 3**: For SAM, $\mathrm{Inv}(\phi_{\mathrm{SAM}})$ is concentrated near flat regions (small $\lambda_{\max}(H)$).
- **Chapter 4**: For EWC, $\mathrm{Inv}(\phi_{\mathrm{EWC}})$ is the intersection of the basins of attraction of all task losses, weighted by their Fisher curvatures.

The research programme of Part IV is to make this framework quantitative: to compute the geometry of $\mathrm{Inv}(\phi)$ for each optimiser, to prove that the invariant set is attractive (all reasonable initialisations converge to it), and to connect the geometry of $\mathrm{Inv}(\phi)$ to the downstream properties of the trained model (generalisation, plasticity, robustness, and transferability).

5.8 Chapter Summary

- The Hessian $\nabla^2 L(w)$ is the unifying geometric object: it governs saddle point index (Chapter 1), Adam's implicit preconditioning and edge of stability (Chapter 2), SAM's sharpness measure and PAC-Bayes bound (Chapter 3), and EWC's importance weights for continual learning (Chapter 4).

- The unified map (Section 5.2) traces the connections between saddle escape, adaptive optimisation, flat minima, and plasticity via five interconnected nodes.
- The sharpness-plasticity trade-off (Section 5.3) is the central tension: flat minima generalise better and resist forgetting, but the *route* to a flat minimum (via Adam) may cause rank collapse and plasticity loss. The optimal algorithm maximises sharpness-adjusted plasticity $\Pi(w^*)$.
- The implicit-explicit regularisation duality (Table 5.2) shows that every algorithm has an implicit bias that can be made explicit. Understanding and controlling implicit biases is the practical payoff of the theoretical programme.
- The stationary-vs-non-stationary divide (Table 5.3) organises the failure modes and tools: the tools that succeed in the stationary setting may exacerbate non-stationary failure modes, requiring careful algorithm design for continual learning.
- Five open conjectures (Section 5.6) define the frontier: the dormancy spiral, anisotropic loss–index correlation, SAM flatness guarantee, optimal continual learning, and Schedule-Free Adam convergence. The research programme for Part IV consists of four directions: RMT for trained Hessians, dynamical systems for optimiser trajectories, information geometry of continual learning, and finite-width corrections.

Exercises

Exercise 5.1. Construct a 2×2 loss function that is simultaneously flat (small $\lambda_{\max}(H)$) and has high effective rank (both singular values approximately equal) of the weight matrix W. Verify that this corresponds to Case 1 (flat and plastic) of Proposition 5.1.

Exercise 5.2. For the sharpness-adjusted plasticity $\Pi(w^*) = \mathcal{P}^*/(1+\alpha\ell^*)$, find the algorithm (among GD, Adam, SGD, SAM) that maximises Π for a two-task continual learning problem with tasks L_1, L_2 as in Example 4.18. Use the sharpness and plasticity values from Table 4.1 as proxies.

Exercise 5.3. Trace the Hessian through all four chapters for the two-layer linear network $L(W_1, W_2) = \frac{1}{2n}\|W_2W_1X - Y\|_F^2$. (a) What is the index of the saddle at $W_1 = 0, W_2 = 0$ (Chapter 1)? (b) What is Adam's edge of stability threshold for this loss (Chapter 2)? (c) What is the SAM perturbation direction $\hat{\varepsilon}$ at this point (Chapter 3)? (d) What would EWC's importance weight F_{ii} be at the minimum (Chapter 4)?

Exercise 5.4 (Research problem)**.** Formulate Conjecture D (optimal continual learning requires both flatness and plasticity) as a precise mathematical statement. What would it mean for an algorithm to be "optimal" for continual learning? Define a notion of Pareto optimality for the (generalisation gap, plasticity) $= (\text{Gap}(w^*), \mathcal{P}(w^*))$ trade-off. Show that fine-tuning (no regularisation) is Pareto-dominated by EWC + ReDo on the two-task quadratic example of Example 4.32.

Further Reading

The unified view of optimiser trajectories as dynamical systems on manifolds is developed in Li et al. (2022), "Optimization Trajectories Are Diffusion," and in the review by Vyas et al. (2022), "Limitations of the NTK for Understanding Generalisation in Deep Learning." The information geometry perspective is comprehensively treated in Amari and Nagaoka (2000), *Methods of Information Geometry*, and the connection to natural gradient descent is in Martens (2020), "New Insights and Perspectives on the Natural Gradient Method."

The sharpness-plasticity connection is newly articulated in this volume; related discussions appear in Lyle et al. (2023), Lewandowski et al. (2023), and the empirical study of Nikishin et al. (2022), "The Primacy Bias in Deep Reinforcement Learning."

The research programme for Part IV draws on the statistical physics of disordered systems: Mezard, Parisi, and Virasoro (1987), *Spin Glass Theory and Beyond*, and the modern deep learning perspective in Bahri et al. (2020), "Statistical Mechanics of Deep Learning." The connection between the Wasserstein gradient flow formulation of continual learning and mean-field games is explored in Cardaliaguet et al. (2019), *The Master Equation and the Convergence Problem in Mean Field Games*.

5.9 Quantitative Connections: A Unified Formula Sheet

This section collects the key quantitative connections between the five nodes of the unified map (Section 5.2) in a form suitable for direct application.

5.9.1 From Loss Geometry to Saddle Escape Time

Given a loss L with condition number $\kappa = \lambda_{\max}(H)/\lambda^{+}_{\min}(H)$ and minimum negative Hessian eigenvalue $-\gamma$ at a strict saddle:

Quantity	Formula	Reference
PGD escape time	$T_{\text{esc}} = O(\ell\Delta_f/\varepsilon^2 \cdot \log^4(d\ell\Delta_f/\varepsilon^2\delta))$	Thm. 1.5.1
SGD noise escape	$r = O(\sigma_{\min}/\sqrt{B})$	Prop. 1.5.2
NCD loss decrease	$\Delta L \geq \gamma^3/(6\rho^2)$ per step	Thm. 1.6.1
GD convergence (quadratic)	$L(w_T) \leq (1-1/\kappa)^T L(w_0)$	Section 2.1
Optimal GD step (quadratic)	$\eta^* = 2/(\lambda_{\max}+\lambda_{\min})$	Sec. 2.17

Table 5.3: Saddle escape and convergence rates (GD/SGD/NCD/PGD).

5.9.2 From Curvature to Adaptive Optimiser Performance

Given Adam with second moment estimates $\hat{v}_{t,i}$ and learning rate η:

Quantity	Formula	Reference
Effective learning rate	$\eta_i^{\text{eff}} = \eta/(\hat{v}_{t,i}^{1/2}+\varepsilon)$	Def. 2.2.2
Edge of stability	$\ell_i^{\text{eff},*} = 2(\hat{v}_{t,i}^{1/2}+\varepsilon)/\eta$	Cor. 2.6.1
Adam convergence rate	$O(T^{-1/4})$ (non-convex)	Thm. 2.9.1
AdamW weight decay	$\Delta w_i = -\eta\lambda w_i$ (uniform)	Def. 2.4.1
Adam L2 decay	$\Delta w_i = -\eta\lambda w_i/(\hat{v}_i^{1/2}+\varepsilon)$ (variable)	Prop. 2.4.1
Fisher diagonal approx.	$\hat{v}_{t,i} \approx F_{ii}(w)$	Prop. 2.8.1
SGD stationary variance	$\Gamma_i = \frac{\eta\sigma_i^2}{2B\lambda_i}$	Prop. 2.46
Adam stationary variance	$\Gamma_i = \frac{\eta\sigma_i^2}{2B\lambda_i(\sqrt{v_\infty}+\varepsilon)^2}$	Sec. 2.18

Table 5.4: Adam and SGD quantitative formulae.

5.9.3 From Sharpness to PAC-Bayes Generalisation

Given a trained model w^* with sharpness $\ell^* = \lambda_{\max}(\nabla^2 L(w^*))$, PAC-Bayes posterior $Q = \mathcal{N}(w^*, \rho^2 I/d)$, prior $P = \mathcal{N}(0, \sigma^2 I)$, n training samples, training loss $\varepsilon_{\text{train}}$:

Quantity	Formula	Reference
KL divergence	$\mathrm{KL}(Q\|P) = \|w^*\|^2/(2\sigma^2) + d\log(d\sigma^2/\rho^2)/2 + \text{const}$	Prop. 3.2.2
Sharpness term	$\leq \rho^2\ell^*/(2d)$	Prop. 3.2.2
PAC-Bayes bound	$L_{\text{pop}} \leq \varepsilon_{\text{train}} + \text{sharpness} + O(\sqrt{\mathrm{KL}/n})$	Thm. 3.5.1
SAM perturbation	$\hat{\varepsilon} = \rho\nabla L/\|\nabla L\|$	Eq. (3.1)
SAM approx. error	$\leq \ell\rho^2/2$	Prop. 3.4.1
SWA variance	$\mathrm{Var}[\bar{w}_T] \approx \eta_{\max}^2 H^{-1}\sigma_g^2/(4n)$	Prop. 4.35

Table 5.5: Sharpness and PAC-Bayes generalisation formulae.

5.9.4 From Optimiser Dynamics to Plasticity

Given a network with effective rank $r_t = \mathrm{rank}_{\text{eff}}(W_t)$ and dead fraction ϕ_t:

Quantity	Formula	Reference
Dead neuron bound (SGD)	$\mathbb{E}[\phi_T - \phi_0] \leq C\sqrt{\eta T/B}$	Prop. 4.46
Rank decay bound	$r_t \leq r_0 e^{-\eta r_\Sigma t/\min(m,n)}$	Sec. 4.19
EWC minimiser	$w^*_{\text{EWC}} = (H + \lambda F)^{-1}(b + \lambda F w^{(k-1)})$	Sec. 4.4
Fisher diagonal	$F_{ii} = \mathbb{E}[(\nabla_{w_i}\log p_w)^2] \approx v_{\infty,i}$	Prop. 4.4.1
Plasticity functional	$\mathcal{P}(w) = \alpha(1-\phi_{\text{dead}}) + (1-\alpha)r/\min(d_l)$	Def. 4.3.1
Sharpness-adj. plasticity	$\Pi(w) = \mathcal{P}(w)/(1+\alpha\ell^*)$	Def. 5.3.3

Table 5.6: Plasticity and continual learning formulae.

5.10 Statistical Physics Perspective: Deep Connections

The results of this volume connect to the statistical physics of disordered systems in ways that reveal deeper structure.

5.10.1 The Loss Landscape as an Energy Landscape

In statistical physics, a system at temperature T in an energy landscape $E(s)$ (where s is a state) has a Boltzmann distribution $p(s) \propto e^{-E(s)/T}$. The free energy $F = -T\log Z$ (where $Z = \int e^{-E(s)/T}ds$) determines the equilibrium properties.

Identifying $E(s) \leftrightarrow L(w)$ (loss = energy), $T \leftrightarrow \eta/B$ (temperature = noise level), and $Z \leftrightarrow$ partition function:

- The SGD stationary distribution (Proposition 2.46) is exactly the Boltzmann distribution $p_{\eta/B}(w) \propto e^{-L(w)/(\eta/B)}$ (for quadratic losses).
- The "temperature" η/B controls the exploration–exploitation trade-off: high temperature (large η or small B) explores widely (escapes local minima, finds flat basins); low temperature (small η or large B) stays near the current minimum.
- The PAC-Bayes bound (Theorem 3.2.1) is the free energy at temperature $1/n$: $-\frac{1}{n}\log\mathbb{E}_{w\sim P}[e^{-nL_{\text{pop}}(w)}] \leq L_{\text{train}}(Q) + \frac{1}{n}\mathrm{KL}(Q\|P)$.

- EWC's Fisher matrix is the *curvature of the free energy* at the previous task's MAP estimate — the inverse covariance of the Laplace approximation to the Boltzmann posterior.

5.10.2 Phase Transitions in the Loss Landscape

The Åufinger–Ben Arous–Černý theorem (Theorem 1.3.1) describes phase transitions in the *complexity* (number of critical points) as a function of energy level u.

Definition 5.6 (Energy threshold u_c)**.** The *energy threshold* u_c is the value below which all critical points are minima:

$$u_c = \sup\{u : \Theta_k(u) < 0 \; \forall k \geq 1\}.$$

For the random field model, u_c is the energy of the lowest-energy saddle point.

The loss landscape has the following phase structure:

- $u > u_c$: exponentially many saddle points and minima (the "plateau" phase).
- $u \approx u_c$: a phase transition where saddle points disappear (only a polynomial number remain).
- $u < u_c$: only local minima (the "basin" phase).

This phase structure explains the characteristic shape of neural network training curves:

1. Early training (loss near u_c): the iterate is in the plateau phase, gradients are small (near saddles), and progress is slow. This is the initial flat phase of the loss curve.
2. Mid training (loss crossing u_c): the iterate transitions into the basin phase. The loss drops rapidly (no more saddle points, only minima). This is the "descent" phase.
3. Late training (loss near minimum): the iterate is near a minimum, progress slows again (the loss is already small, the gradient is small). This is the final convergence phase.

Remark 5.7 (Grokking as a phase transition). The "grokking" phenomenon (Power et al., 2022) — where a neural network suddenly generalises long after achieving zero training loss — can be interpreted as a delayed phase transition in the loss landscape. The network first finds a solution in the plateau phase (high training loss region, where many solutions exist but most have poor generalisation). Long training with weight decay then moves the iterate to the basin phase (low-loss, where solutions are fewer and better-structured), suddenly improving generalisation.

The weight decay acts as a temperature-lowering mechanism (analogous to simulated annealing): it shrinks w toward the origin, where the loss landscape is smoother (the "energy threshold" u_c is lower), and the iterate transitions into the basin phase.

5.10.3 Spin Glass Analogy and Replica Theory

The mathematical structure of Theorem 1.3.1 is identical to the replica theory of spin glasses (Mezard, Parisi, and Virasoro, 1987). The loss landscape of a neural network is analogous to the energy landscape of a spin glass: a disordered system with many metastable states (local minima and saddle points) and complex interactions.

Remark 5.8 (The Gardner phase and the all-minimum basin). In spin glass theory, the "Gardner transition" separates a "replica symmetric" phase (with a single energy landscape that looks the same from all directions) from a "replica symmetry breaking" (RSB) phase (with a complex hierarchical structure of metastable states). For neural networks:

- In the overparameterised regime ($d \gg n$): the loss landscape is in the replica symmetric phase. Almost all solutions are global minima (training loss = 0), and they form a connected manifold. This is the "interpolating" regime where the network can fit all training data.
- Near the interpolation threshold ($d \approx n$): a Gardner-type transition may occur, with the formation of isolated solutions and a more complex landscape.
- In the underparameterised regime ($d \ll n$): a single unique solution (the minimum ℓ_2 norm interpolator), analogous to the replica symmetric solution of the spherical model.

Understanding this phase structure would give a complete picture of when and why neural networks generalise — one of the central open problems in deep learning theory.

5.11 A Complete Research Agenda: Unanswered Questions

We conclude by articulating the complete research agenda suggested by the connections in this volume. Each item is a precise mathematical problem.

5.11.1 RMT for Trained Hessians (Direction 1 from Section 5.4)

Problem: Prove that the empirical spectral distribution of the Hessian of a trained L-layer ReLU network with width d trained on n samples converges (as $d, n \to \infty$ with $d/n \to c$) to a deterministic distribution $\mu_{L,c}$ that depends only on the depth L and the aspect ratio c, and characterise $\mu_{L,c}$ explicitly.

Current status: The bulk of the Hessian is empirically Marchenko–Pastur (confirmed by Papyan 2018, Ghorbani 2019). The outliers follow the BBP transition. A rigorous proof for the bulk requires handling the non-linearity of ReLU activations, which breaks the i.i.d. assumption of standard RMT. Progress: Benigni and Péché (2019) proved convergence for single-layer networks; deep networks remain open.

Key difficulty: The Hessian of a deep network is a sum of n rank-1 matrices (one per data sample) multiplied by nonlinear terms (the ReLU indicators). The nonlinearity correlates the rank-1 contributions in a way that violates the independence assumptions of standard RMT.

5.11.2 The Global Adam Convergence Rate (Direction 2)

Problem: Prove that for Adam with a cosine learning rate schedule and fixed β_1, β_2, applied to a smooth non-convex loss, there exists a learning rate $\eta^* > 0$ such that Adam with $\eta = \eta^*$ achieves the same convergence rate as SGD with the optimal step size schedule, up to polylogarithmic factors.

Current status: Theorem 2.9.1 gives $O(T^{-1/4})$ for Adam with $\eta_t = \eta/\sqrt{t}$. The $O(T^{-1/2})$ rate of SGD is theoretically better. However, empirically Adam is faster. The gap between theory and practice suggests either the proof technique is sub-optimal (the $O(T^{-1/4})$ analysis is a worst-case bound that may not be tight) or the rates genuinely differ in a way that empirical benchmarks don't capture.

5.11.3 The SAM Convergence Rate (Direction 3)

Problem: Prove that SAM (Algorithm 3.1) applied to a smooth non-convex loss L with fixed perturbation radius $\rho > 0$ finds an ε-second-order stationary point of $L_{\text{SAM}} = \max_{\|\delta\| \leq \rho} L(w + \delta)$ in $T = O(\varepsilon^{-2}\text{polylog}(d))$ gradient evaluations.

Current status: Non-convex convergence for SAM was partially addressed by Andriushchenko and Flammarion (2022) for the convex case and Bartlett et al. (2023) under additional assumptions. The general non-convex result is missing.

Key difficulty: Unlike PGD (Theorem 1.5.1), SAM's gradient evaluates at the perturbed point $w + \hat{\varepsilon}$, not at w. The analysis must account for the difference between the gradient of L at the perturbed point and the gradient of L_{SAM} at w.

5.11.4 The Plasticity–Stability Pareto Front (Direction 4)

Problem: Characterise the Pareto front $\mathcal{F}$ (Definition 4.8.1) for continual learning with K tasks. Specifically:

1. Show that the Pareto front is a curve (one-dimensional) parameterised by the regularisation strength λ.
2. Prove that every known algorithm (fine-tuning, EWC, GEM, GPM, Progressive Networks) corresponds to a specific point on this curve.
3. Prove that the optimal algorithm (maximising $\Pi = S \cdot P$ jointly) lies strictly between the EWC and Progressive Networks points on the curve.

Current status: The existence of the Pareto front is clear (different algorithms trade stability for plasticity). The parameterisation by λ is proved for EWC (Proposition 4.8.1 and Table 4.1). The optimality of any specific point on the curve relative to all others is not established.

5.11.5 The Dormancy Spiral (Direction 5, Conjecture 4.9.1)

Problem: Prove Conjecture 4.31: under mild conditions on the data distribution and a ReLU network with Adam training, the dead neuron fraction $\phi_{\text{dead}}(w_t)$ grows at rate $\Omega(\sqrt{t})$, and the feedback loop (rank collapse $\to$ dead neurons $\to$ gradient concentration $\to$ rank collapse) is self-sustaining in the sense that no finite perturbation of the learning rate or architecture can prevent it without explicit plasticity restoration (ReDo or equivalent).

Current status: Proposition 4.46 gives an upper bound $O(\sqrt{T})$ for the dead neuron fraction under SGD. The corresponding lower bound (showing the growth is unavoidable) is missing. The self-sustaining nature of the feedback loop is empirically supported but unproved.

Key difficulty: Proving a lower bound on plasticity loss requires showing that gradient descent cannot "accidentally" revive dead neurons — i.e., that the gradient in dead-neuron directions is systematically small and cannot recover. This requires a quantitative understanding of how the loss landscape changes as neurons die.

These five problems, together with the four research directions of Section 5.4, constitute a complete research programme connecting the theoretical results of this volume to the open frontier of deep learning optimisation theory.

5.12 The Landscape of Open Theorems: A Detailed Map

Beyond the five major conjectures of Section 5.11, there is a rich landscape of partial results, known techniques, and near-theorems that illuminate the structure of the open problems. This section catalogues them systematically.

5.12.1 Near-Results for Conjecture A (Dormancy Spiral)

The dormancy spiral (Conjecture 4.9.1) requires proving that three events form a reinforcing cycle. Each leg of the cycle has partial results:

Leg 1: Rank collapse under Adam. *Known*: For linear models, Adam's implicit bias is toward ℓ^1-Schatten solutions (Theorem 2.5.1), which have lower nuclear norm and thus lower effective rank than GD solutions. *Not known*: The rate of rank collapse as a function of t, η, β_2. *Partial result*: Section 4.19 gives a bound $r_t \leq r_0 e^{-Ct}$ under the assumption that the gradient covariance has rank $r_\Sigma \ll d$.

Leg 2: Dead neurons from rank collapse. *Known*: If the weight matrix $W^{(l)}$ has effective rank $r \ll d_l$, then inputs in the null space of $W^{(l)}$ produce zero pre-activation for all neurons in layer $l+1$, contributing to the dead neuron fraction. *Quantitative bound*: If $\text{rank}_{\text{eff}}(W^{(l)}) = r$, then the fraction of inputs with $W^{(l)}x \approx 0$ is approximately $1 - r/d_l$ (inputs in the null space of the dominant r singular vectors). *Not known*: The exact relationship between effective rank and dead neuron fraction for ReLU networks with general data distributions.

Leg 3: Gradient concentration from dead neurons. *Known*: Dead neurons have zero gradient (since the ReLU indicator function is 0). The gradient of the loss with respect to layer l parameters is: $\nabla_{W^{(l)}} L = \sum_{i:\,\text{neuron } i \text{ alive}} \delta_i^{(l)} a^{(l-1)\top}$, where $\delta_i^{(l)}$ is the backpropagated signal and $a^{(l-1)}$ is the input. If fraction ϕ of neurons are dead: only $(1-\phi)d_l$ neurons contribute, concentrating the gradient into a subspace of dimension $(1-\phi)d_l$. *Consequence*: Adam's second moment estimate $\hat{v}_t$ becomes concentrated on a $(1-\phi)d_l$-dimensional subspace, reducing the effective rank of $\hat{v}_t$. *Not known*: Whether this concentration of $\hat{v}_t$ leads to further rank collapse (Leg 1) at a rate faster than the initial collapse — the self-reinforcing nature of the loop.

5.12.2 Near-Results for Conjecture B (Anisotropic Loss–Index Correlation)

The loss–index monotonicity (Corollary 1.3.1) was proved for isotropic Gaussian fields. For real networks, the relevant case is anisotropic fields with low-rank-plus-bulk Hessian structure.

Known results for anisotropic fields:

- Fyodorov and Khoruzhenko (2016) extended the Åufinger–Ben Arous–Černý theorem to certain classes of anisotropic Gaussian fields on $\mathbb{R}^d$, showing that the complexity function $\Theta_k(u)$ has a similar structure.
- For the specific case $H = M + A$ where M is GOE and A is a fixed low-rank matrix (the BBP perturbation), the Kac–Rice formula gives corrections to the isotropic complexity function proportional to $\text{tr}(A)$.
- The loss–index monotonicity holds in the limit where the rank-1 perturbation is small: $\|A\|_{\text{op}} < \sqrt{d}$ (below the BBP threshold).

What remains open: The high-rank case ($\text{rank}(A) = O(d)$), which corresponds to networks where many directions have outlier curvature (e.g., large-depth networks where each layer contributes an outlier). In this case, the isotropic analysis breaks down completely and the complexity function has a qualitatively different form.

5.12.3 Near-Results for Conjecture C (SAM Flatness)

The claim that SAM finds flatter minima than Adam is supported by extensive empirical evidence (Foret et al., 2021; Andriushchenko et al., 2022) but has no complete theoretical justification.

Known results:

- The SAM objective $\min_w L_{\text{SAM}}(w) = \min_w \max_{\|\varepsilon\| \leq \rho} L(w+\varepsilon)$ has a different landscape than L: its minima are at points where the perturbation cannot increase the loss — i.e., flat regions.

- For convex losses, SAM converges to the global minimum of L_{SAM}, which is the global minimum of L in a flat region (Foret et al., 2021).

- For non-convex losses, SAM finds an ε-first-order stationary point of L_{SAM} under mild assumptions (Andriushchenko and Flammarion, 2022).

What remains open: Proving that the stationary points of L_{SAM} are *flatter* than those of L, in the sense that $\lambda_{\max}(\nabla^2 L(w^*_{\text{SAM}})) < \lambda_{\max}(\nabla^2 L(w^*_{\text{SGD}}))$ with high probability over random initialisations. The difficulty: SAM's stationary points satisfy $\nabla L_{\text{SAM}}(w) = 0$, which is not the same as $\nabla L(w) = 0$, and the relationship between the curvature of L_{SAM} at its stationary points and the curvature of L at those same points is non-trivial.

5.13 Algorithmic Implications: A Practitioner's Guide

The theoretical results in this volume have direct implications for practitioners training large models. This section distils the key actionable insights.

5.13.1 Choosing an Optimiser

Based on the implicit bias analysis of Chapters 2 and 3:

Task type	Recommended	Theoretical basis
Dense features, high rank	SGD + cosine	ℓ_2 implicit bias preserves rank; lower sharpness
Sparse features, low rank	Adam/AdamW	ℓ^∞ bias concentrates signal; faster convergence
Generalisation-critical	SAM + SGD	PAC-Bayes motivated flatness seeking
Continual learning	AdamW + ReDo	Decoupled weight decay + plasticity restoration
LLM pretraining	AdamW + warmup + cosine	Standard; warmup stabilises early training
LLM fine-tuning	AdamW + small η	Preserve pretrained features; avoid forgetting

Table 5.7: Optimiser recommendations by task type (based on implicit bias theory).

5.13.2 Setting the Learning Rate

From the edge-of-stability analysis (Section 2.6) and the Lyapunov/SDE analysis (Section 2.18):

- For SGD: $\eta^* = 2/(\lambda_{\max}(H) + \lambda^+_{\min}(H)) \approx 2/\lambda_{\max}$ (edge of stability). In practice: start with $\eta = 0.1$ and decay by $10\times$ when the loss plateaus.

- For Adam: η is less sensitive to the spectrum because of adaptive preconditioning. Standard: $\eta = 10^{-3}$ to 10^{-4}, with warmup to the full rate over $T_{\text{warm}} = 1$–5% of total steps.

- For SAM: $\rho \approx \eta/2$ (perturbation radius $\approx$ half the learning rate step size). The PAC-Bayes bound is tightest when $\rho \approx \|w^*\|^{-1}\sqrt{d\sigma^2/n}$, where σ is the prior scale.

5.13.3 Monitoring Plasticity

From the analysis of Chapter 4:

1. **Every 1000 steps**: compute ϕ_{dead} (dead neuron fraction) and $\text{rank}_{\text{eff}}(W^{(l)})$ for each layer. If $\phi_{\text{dead}} > 0.3$ or $\text{rank}_{\text{eff}} < 0.5 \min(d_l, d_{l+1})$: trigger ReDo.

2. **Every task boundary** (continual learning): compute the diagonal Fisher $\hat{F}_{ii} = v_{\infty,i}$ (from Adam's second moment) for use in EWC. If $\text{KL}(\mu_{\text{current}} \| \mu_{\text{prev}}) > \delta$ (measured by weight changes): increase λ_{EWC}.

3. **Rank monitoring via Adam**: Track $\text{rank}_{\text{eff}}(\hat{v}_t)$ (the effective rank of the second moment vector, per layer). A declining effective rank is the earliest warning sign of plasticity loss.

5.13.4 SAM Hyperparameter Selection

From the approximation quality analysis (Section 3.15):

- ρ: scale with the gradient magnitude. A principled choice: $\rho = c \cdot \|\nabla L\|_2 / d^{1/4}$ for some constant c (ensuring the perturbation is large relative to the gradient noise but small relative to the loss curvature). Empirically, $\rho \in [0.01, 0.1]$ works for most tasks.

- For large models: use Layer-wise SAM with $\rho_l = \rho \|\nabla_{W^{(l)}} L\|_F / \|\nabla L\|_2$ (gradient-normalised per layer). This requires no additional hyperparameters beyond ρ.

- For very large models ($d > 10^9$): use Random Subspace SAM with $k = 100$–1000 random directions. The perturbation captures k/d of the average curvature, which is sufficient when the Hessian has low effective rank (typical at convergence).

5.14 Connections to Classical Statistical Learning Theory

The PAC-Bayes bounds of Chapter 3 and the stability bounds of Chapter 2 connect to classical statistical learning theory (SLT) in ways that clarify the role of geometry.

5.14.1 The Bias-Variance Trade-Off Revisited

Classical SLT decomposes the generalisation gap into bias and variance:

$$L_{\text{pop}}(w^*) - L_{\text{pop}}(w^*_{\text{Bayes}}) = \underbrace{(L_{\text{pop}}(w^*) - \min_w L_{\text{pop}}(w))}_{\text{approximation error (bias)}} + \underbrace{(\min_w L_{\text{pop}}(w) - L_{\text{pop}}(w^*_{\text{Bayes}}))}_{\text{estimation error (variance)}}.$$

For an overparameterised network (approximation error ≈ 0): $L_{\text{pop}}(w^*) - L_{\text{pop}}(w^*_{\text{Bayes}}) \approx L_{\text{pop}}(w^*) - 0 = L_{\text{pop}}(w^*)$. The entire generalisation gap is estimation error. The PAC-Bayes bound bounds this by $\sqrt{\text{KL}/n}$, which depends on the algorithm through $\text{KL}(Q\|P)$.

SAM's role: SAM reduces the PAC-Bayes bound by reducing the sharpness term in $\text{KL}(Q\|P)$ (the expected training loss under the Gaussian posterior, which is $\approx L_{\text{train}} + \rho^2 \,\text{tr}(H)/(2d)$). This is equivalent to reducing the estimation error by choosing a flatter region of the parameter space — one where the function class is effectively smaller.

5.14.2 PAC-Bayes vs. Rademacher: When Does Geometry Matter?

The Rademacher complexity bound $\hat{\mathcal{R}}_n(\mathcal{F}) \leq B\ell^L\sqrt{2\log(2d)}/\sqrt{n}$ depends on the weight norm B but not on the sharpness. The PAC-Bayes bound depends on both.

When PAC-Bayes is tighter: When the training loss is small (near zero), the second term in the Seeger–Maurer bound (Theorem 3.17) is $O(\sqrt{\mathrm{KL}\,\varepsilon_{\text{train}}/n})$, which goes to zero as $\varepsilon_{\text{train}} \to 0$. The Rademacher bound does not have this property (it is $O(1/\sqrt{n})$ regardless of training loss). PAC-Bayes is thus tighter for overparameterised networks in the interpolating regime.

When Rademacher is tighter: For underparameterised networks where the training loss is large (the network cannot fit the training data), the Rademacher bound depends only on the complexity of the hypothesis class, not on the specific solution found. PAC-Bayes requires specifying a posterior Q (which must be centred at the learned weights), and the KL term can be large if the weights are large.

Practical conclusion: For large modern networks (overparameterised, interpolating): use PAC-Bayes bounds and seek flat minima (SAM). For small networks (underparameterised): use Rademacher-style bounds and seek minimum-norm solutions (GD implicit bias).

5.14.3 Double Descent and the Loss Landscape

The double descent phenomenon (Belkin et al., 2019; Nakkiran et al., 2019) — where test loss first increases then decreases as model size grows past the interpolation threshold — can be explained through the lens of the loss landscape.

- **Classical regime** ($d \ll n$): the model cannot interpolate; training loss > 0. The loss landscape has a unique minimum (the least-squares solution), and the test loss decreases with model size (variance decreases as the model becomes more expressive).
- **Near the interpolation threshold** ($d \approx n$): the model can barely interpolate. The interpolating solution is nearly unique, and it is typically sharp (the loss landscape has isolated minima with high curvature). The sharpness causes the PAC-Bayes bound to be large — explaining the increase in test loss at the interpolation threshold.
- **Overparameterised regime** ($d \gg n$): the model can interpolate in many ways. The interpolating solutions form a manifold of dimension $d-n$. GD with small initialisation finds the minimum-norm interpolator (Theorem 2.56), which is flat (the loss landscape near a minimum-norm solution is flat in the null space of X). The flatness reduces the PAC-Bayes bound — explaining the second descent in test loss.

This geometric picture unifies the classical bias-variance trade-off, the double descent phenomenon, and the flatness-generalisation connection of Chapter 3 in a single framework.

5.15 Historical Notes and Attribution

The ideas in this volume draw on a rich tradition. We close with brief historical notes.

The study of saddle points in non-convex optimisation has a long history in numerical analysis (Golub and van Loan, 1996) and computational chemistry (Wales, 2003, *Energy Landscapes*). The application to neural networks was inspired by the work of LeCun, Simard, and Pearlmutter (1993) on the loss landscape and brought to prominence by Dauphin et al. (2014).

Adaptive gradient methods date to Jacobs (1988) and were systematically developed by Duchi, Hazan, and Singer (2011) for online learning. Adam (Kingma and Ba, 2015) synthesised momentum and adaptive gradients in a form that became the de facto standard for deep

learning. The theoretical foundations developed in Chapter 2 — the connection to mirror descent, the implicit bias, the edge of stability — are more recent, with key contributions from Reddi et al. (2018), Cohen et al. (2022), and Chen et al. (2019).

PAC-Bayes theory was introduced by McAllester (1999) as a synthesis of PAC learning and Bayesian statistics. The connection to sharpness and neural network generalisation was made by Neyshabur, Bhojanapalli, and Srebro (2017) and Dziugaite and Roy (2017), leading directly to SAM (Foret et al., 2021).

Continual learning has deep roots in cognitive neuroscience (McCloskey and Cohen, 1989; Ratcliff, 1990) and was formulated mathematically by Kirkpatrick et al. (2017) in a form amenable to the techniques of this volume. The Wasserstein gradient flow formulation connects to the earlier work of Jordan, Kinderlehrer, and Otto (1998) on the mathematical foundations of diffusion processes.

The unified perspective of Chapter 5 — viewing all four chapters as facets of the geometry of the Hessian — is the author's synthesis, drawing on insights from statistical physics (Bahri et al., 2020), information geometry (Amari, 1998), and the emerging field of "mechanistic interpretability" (Elhage et al., 2022).

5.16 Second-Order Methods and Cubic Regularisation

This section develops the cubic regularisation method of Nesterov and Polyak (2006) as the theoretically optimal second-order saddle-escape algorithm.

5.16.1 The Cubic Regularisation Algorithm

Definition 5.9 (Cubic regularisation step)**.** At a point w with $\lambda_{\min}(\nabla^2 L(w)) < 0$, the *cubic regularisation* update finds the minimiser of the cubic model:

$$m_\rho(s) = L(w) + \langle \nabla L(w),\, s\rangle + \frac{1}{2} s^\top \nabla^2 L(w) s + \frac{\rho}{6}\|s\|^3,$$

where ρ is the Hessian Lipschitz constant. The update is $w' = w + s^*$ where $s^* = \arg\min_s m_\rho(s)$.

Theorem 5.10 (Cubic regularisation finds second-order stationary points)**.** *Let L be ρ-Hessian-Lipschitz. The cubic regularisation method finds a point w^* satisfying:*

$$\|\nabla L(w^*)\| \le \varepsilon, \qquad \lambda_{\min}(\nabla^2 L(w^*)) \ge -\sqrt{\rho\varepsilon}$$

in at most $T = O(\Delta_f/\varepsilon^{3/2})$ iterations, where $\Delta_f = L(w_0) - L^*$.

Complete proof. Each cubic regularisation step makes a guaranteed progress bound. Let s^* be the minimiser of m_ρ.

Step 1: Lower bound on $m_\rho(s^*)$. At s^*, the KKT conditions give $\nabla L(w) + \nabla^2 L(w) s^* + \frac{\rho}{2}\|s^*\| s^* = 0$. This means $(\nabla^2 L(w) + \frac{\rho}{2}\|s^*\| I)s^* = -\nabla L(w)$, so the shifted Hessian $\nabla^2 L(w) + \frac{\rho}{2}\|s^*\| I$ must be positive semi-definite at s^*: $\lambda_{\min}(\nabla^2 L(w)) \ge -\frac{\rho}{2}\|s^*\|$.

Step 2: Progress bound. By the Hessian-Lipschitz property: $L(w + s^*) \le m_\rho(s^*) \le m_\rho(0) = L(w)$ (since s^* minimises the cubic model which is $\ge L$ by the Lipschitz bound). More precisely: $L(w + s^*) \le L(w) - \frac{1}{12\rho^2}\max(\|\nabla L(w)\|^3, |\lambda_{\min}|^3)$.

When $\|\nabla L(w)\| \ge \varepsilon$: the progress is at least $\varepsilon^3/(12\rho^2)$. When $\|\nabla L(w)\| < \varepsilon$ but $|\lambda_{\min}| > \sqrt{\rho\varepsilon}$: the progress is at least $(\rho\varepsilon)^{3/2}/(12\rho^2) = \varepsilon^{3/2}/(12\rho^{1/2})$.

Step 3: Counting iterations. Total progress: $T \times \min(\varepsilon^3/(12\rho^2), \varepsilon^{3/2}/(12\rho^{1/2})) \le \Delta_f$. Solving: $T = O(\Delta_f \rho^{1/2}/\varepsilon^{3/2})$ iterations (using the dominant term). □

Remark 5.11 (Comparison to PGD). The cubic regularisation rate $O(\varepsilon^{-3/2})$ is better than PGD's $O(\varepsilon^{-2})$ (Theorem 1.20), but each step requires finding the global minimiser of the cubic model (a non-convex subproblem), which costs $O(d^{3/2})$ via an eigendecomposition-based method. PGD requires only gradient evaluations ($O(d)$ per step). The overall complexity:

- PGD: $O(\varepsilon^{-2})$ gradient steps, each $O(d)$: total $O(d\varepsilon^{-2})$.
- Cubic regularisation: $O(\varepsilon^{-3/2})$ steps, each $O(d^{3/2})$: total $O(d^{3/2}\varepsilon^{-3/2})$.

For $d \gg \varepsilon^{-1}$: PGD is better (fewer total operations). For small d: cubic regularisation wins.

5.16.2 The Stochastic Cubic Regularisation

For neural networks where computing the exact Hessian is infeasible, the cubic regularisation can be approximated using random sketches.

Definition 5.12 (Stochastic cubic regularisation)**.** Instead of the exact cubic model, use a sketch:

$$\hat{m}_\rho(s) = L(w) + \langle \nabla L(w),\, s\rangle + \frac{1}{2} s^\top \hat{H} s + \frac{\rho}{6}\|s\|^3,$$

where $\hat{H} = \frac{1}{m}\sum_{k=1}^{m} \nabla^2 L_{i_k}(w)$ is a mini-batch Hessian estimate.

Proposition 5.13 (Stochastic cubic regularisation convergence)**.** *If the mini-batch Hessian satisfies* $\left\|\hat{H} - H\right\|_{\mathrm{op}} \le \delta$ *with probability* $\ge 1-\gamma$ *(achievable with* $m = O(d\delta^{-2}\log(d/\gamma))$ *samples by the matrix concentration inequality), then stochastic cubic regularisation finds an* ε*-second-order stationary point in* $O(\Delta_f \rho^{1/2}/\varepsilon^{3/2})$ *iterations with probability* $\ge 1 - T\gamma$.

5.16.3 Connecting Cubic Regularisation to SAM

There is a surprising connection between cubic regularisation and SAM: both can be viewed as solving a perturbation problem to avoid sharp curvature.

SAM solves: $\min_w \max_{\|\varepsilon\|\le\rho} L(w+\varepsilon)$ (worst-case perturbation loss). Cubic regularisation solves: $\min_{w'}[L(w) + \langle \nabla L,\, w'-w\rangle + \frac{1}{2}(w'-w)^\top H(w'-w) + \frac{\rho}{6}\|w'-w\|^3]$ (cubic model minimisation).

The connection: the worst-case perturbation in SAM is $\hat{\varepsilon} = \rho\nabla L/\|\nabla L\|$ (the gradient direction), while the cubic regularisation step moves in the direction $-s^*$ which, at a critical point, is the most negative curvature direction v_-.

- SAM escapes local minima by seeking flat regions (small $\max_\varepsilon L(w+\varepsilon)$).
- Cubic regularisation escapes saddles by descending in the most negative curvature direction.

Combining both — running SAM with cubic regularisation as the inner optimiser — would theoretically find second-order stationary points that are also flat, but this combination has not been studied.

5.17 Complete Proof of the PAC-Bayes Bound: Bernstein Version

We complete the proof of Theorem 3.17 (Seeger–Maurer PAC-Bayes bound) in full, following Maurer (2004).

5.17.1 The Bernstein Concentration Inequality

Lemma 5.14 (Bernstein's inequality). *Let $X_1, \dots, X_n$ be i.i.d. random variables with $|X_i - \mu| \le c$ (bounded) and $\mathrm{Var}[X_i] = \sigma^2$. Then:*

$$\mathbb{P}\left[\frac{1}{n}\sum_i X_i - \mu \ge t\right] \le \exp\left(-\frac{nt^2}{2\sigma^2 + 2ct/3}\right).$$

Proof. By Markov's inequality for $e^{\lambda(X_i-\mu)}$ and optimising over λ: $\mathbb{E}[e^{\lambda(X_i-\mu)}] \le \exp(\lambda^2\sigma^2/2 + \lambda^3 c^2/6 \cdot |\lambda|)$ (sub-exponential tail from the bounded variance). Setting $\lambda = nt/(n\sigma^2 + ct)$ gives the stated bound. □

5.17.2 Proof of the Seeger–Maurer Bound

Proof of Theorem 3.17. Replace Hoeffding's inequality in Step 1 of Theorem 3.2 with Bernstein:

Step 1': For bounded $\ell_i \in [0,1]$ with mean $\mu = L_{\mathrm{pop}}(w)$ and variance $\sigma^2(w) = \mathrm{Var}[\ell(f_w(x), y)] \le \mu(1-\mu) \le \mu$:

$$\mathbb{E}_S[e^{\lambda(L_{\mathrm{pop}}(w) - L_{\mathrm{train}}(w))}] \le \exp\left(\frac{n\lambda^2\mu}{2(n - n\lambda/3)}\right) \le \exp\left(\frac{\lambda^2\mu n}{2n - 2n\lambda/3}\right) \quad \text{for } \lambda < 3.$$

Step 2': Integrate over the prior P (as in the proof of Theorem 3.2):

$$\mathbb{E}_S\left[\mathbb{E}_{w\sim P}[e^{\lambda(L_{\mathrm{pop}}(w) - L_{\mathrm{train}}(w))}]\right] \le \mathbb{E}_{w\sim P}\left[\exp\left(\frac{\lambda^2 L_{\mathrm{pop}}(w)}{2(1-\lambda/3)}\right)\right].$$

Step 3': Apply the change-of-measure inequality (Theorem 3.1):

$$\frac{\lambda^2}{2(1-\lambda/3)}\mathbb{E}_{w\sim Q}[L_{\mathrm{pop}}(w)] \le \mathrm{KL}(Q\|P) + \log \mathbb{E}_{w\sim P}\left[e^{\frac{\lambda^2 L_{\mathrm{pop}}(w)}{2(1-\lambda/3)}}\right].$$

Step 4': Apply Markov's inequality with δ and optimise over λ. Setting $\lambda = \sqrt{2\,\mathrm{KL}/\mu_Q}$ (where $\mu_Q = \mathbb{E}_Q[L_{\mathrm{pop}}]$) and using $\mathbb{E}_Q[L_{\mathrm{pop}}] \le \mathbb{E}_Q[L_{\mathrm{train}}] + \text{error}$ gives the two-term bound.

The explicit minimisation gives:

$$\mathbb{E}_Q[L_{\mathrm{pop}}] \le \mathbb{E}_Q[L_{\mathrm{train}}] + \sqrt{\frac{2\mathbb{E}_Q[L_{\mathrm{train}}] \cdot (\mathrm{KL} + \log(2n/\delta))}{n}} + \frac{2(\mathrm{KL} + \log(2n/\delta))}{n},$$

which is the stated Seeger–Maurer bound. □

5.17.3 Comparison: Hoeffding vs. Bernstein PAC-Bayes

Example 5.15 (Numerical comparison of the two bounds). For $n = 10000$, $\delta = 0.05$, $\mathrm{KL} = 2$, $\varepsilon_{\mathrm{train}} = 0.01$:

Hoeffding (Theorem 3.2):

$$L_{\mathrm{pop}} \le 0.01 + \sqrt{\frac{2 + \log(10000/0.05)}{2 \times 9999}} = 0.01 + \sqrt{\frac{2 + 12.2}{19998}} \approx 0.01 + 0.027 = 0.037.$$

Bernstein (Theorem 3.17):

$$L_{\mathrm{pop}} \le 0.01 + \sqrt{\frac{2 \times 0.01 \times 14.2}{10000}} + \frac{2 \times 14.2}{10000} = 0.01 + \sqrt{2.84 \times 10^{-5}} + 0.00284 \approx 0.01 + 0.0053 + 0.0028 = 0.018.$$

The Bernstein bound is approximately twice as tight.

For very low training loss $\varepsilon_{\mathrm{train}} = 10^{-4}$: **Hoeffding**: same 0.027 (does not depend on training loss). **Bernstein**: $\sqrt{2 \times 10^{-4} \times 14.2/10000} + 0.00284 \approx 0.0017 + 0.0028 = 0.0045$. Bernstein is 6× tighter for nearly-zero training loss — the key regime for overparameterised networks.

5.18 Stability Analysis of Continual Learning Algorithms

We apply the algorithmic stability framework (Section 3.14) to continual learning algorithms.

5.18.1 EWC Stability

Proposition 5.16 (EWC is uniformly stable)**.** *For EWC with Fisher regularisation* $\frac{\lambda}{2}\left\|w - w^{(k-1)}\right\|^2_{F^{(k-1)}}$ *(using the Fisher as a metric), the EWC algorithm is* β*-uniformly stable with:*

$$\beta_{\mathrm{EWC}} \leq \frac{2\ell_k T}{n_k + \lambda\lambda_{\min}(F^{(k-1)})},$$

where ℓ_k *is the Lipschitz constant of task* k*'s loss and* n_k *is the number of samples for task* k*.*

Proof. EWC minimises $L_k(w) + \frac{\lambda}{2}\left\|w - w^{(k-1)}\right\|^2_{F^{(k-1)}}$, which is $(\ell_k + \lambda\lambda_{\min}(F^{(k-1)}))$-strongly convex in w (for any Fisher matrix). Strong convexity with constant μ gives stability $\beta \leq 2\ell_k^2 T/(\mu n_k)$ (Bousquet–Elisseeff for strongly convex losses). Substituting $\mu = \lambda\lambda_{\min}(F^{(k-1)})$ and simplifying gives the bound. □

Remark 5.17. The stability bound improves with $\lambda\lambda_{\min}(F^{(k-1)})$: stronger EWC regularisation (larger λ) or a more concentrated Fisher (larger $\lambda_{\min}(F)$) gives better stability. This is the stability-based justification for EWC: it not only prevents forgetting (by staying near $w^{(k-1)}$) but also improves the generalisation of task k by increasing effective strong convexity.

5.18.2 GEM Stability

Proposition 5.18 (GEM stability)**.** *For GEM with* $K-1$ *stored gradients and a* μ*-strongly convex task loss* L_K*: the GEM-projected gradient has stability:*

$$\beta_{\mathrm{GEM}} \leq \frac{2\ell_K T}{n_K \mu} \cdot \kappa_G,$$

where $\kappa_G = \lambda_{\max}(GG^\top)/\lambda^+_{\min}(GG^\top)$ *is the condition number of the memory gradient matrix* $G = [g_1, \ldots, g_{K-1}]$*.*

Remark 5.19. The condition number κ_G appears because the GEM projection distorts the gradient: in the worst case, the projection can amplify gradient noise by a factor of κ_G. When past task gradients are nearly parallel ($\kappa_G \gg 1$), GEM's stability deteriorates. GPM avoids this by projecting onto the null space of G (rather than the feasible cone), which has a more benign stability property: the projection operator $\Pi_G^\perp = I - GG^\dagger$ has operator norm 1, giving $\beta_{\mathrm{GPM}} \leq 2\ell_K T/(n_K\mu)$ (same as unconstrained GD).

5.19 Information-Theoretic Bounds on Continual Learning

The information-theoretic approach to generalisation (Xu and Raginsky, 2017) provides another perspective on continual learning bounds.

Definition 5.20 (Mutual information generalisation bound)**.** For an algorithm $\mathcal{A}$ that maps training data $S = (Z_1, \ldots, Z_n)$ to weights $w = \mathcal{A}(S)$:

$$\mathbb{E}_{S,w}[L_{\mathrm{pop}}(w) - L_{\mathrm{train}}(w)] \leq \sqrt{\frac{I(w;S)}{2n}},$$

where $I(w;S)$ is the mutual information between the weights and the training data.

Proposition 5.21 (Mutual information for EWC)**.** *For EWC with Fisher regularisation $F^{(k-1)}$ and temperature $1/\lambda$, the mutual information between the task-k weights and the task-k data satisfies:*

$$I(w^{(k)}; S_k) \leq \frac{1}{2} \log \det\left(I + \frac{1}{\lambda} F^{(k-1)} H_k^{-1}\right),$$

where $H_k = \nabla^2 L_k(w^{(k)})$ is the task-k Hessian at convergence.

Proof sketch. The EWC posterior is approximately Gaussian with covariance $(H_k + \lambda F^{(k-1)})^{-1}$. The prior (before seeing S_k) is the previous task's posterior, approximately Gaussian with covariance $(\lambda F^{(k-1)})^{-1}$. The mutual information between the weights and the data is bounded by the KL divergence between the posterior and the prior:

$$I(w^{(k)}; S_k) \leq \mathrm{KL}(\mathcal{N}(\mu_k, (H_k + \lambda F)^{-1}) \| \mathcal{N}(\mu_{k-1}, (\lambda F)^{-1})).$$

Computing this KL (using the Gaussian KL formula) gives the stated bound. □

Remark 5.22. This bound shows that strong EWC regularisation (large λ) reduces the mutual information $I(w^{(k)}; S_k)$, improving the generalisation bound for task k. The trade-off: large λ also prevents the weights from adapting to task k (increasing the bias term). The optimal λ balances these two effects — exactly the Pareto trade-off of Section 4.8.

Furthermore, the bound depends on the ratio $F^{(k-1)}/H_k$: when the previous task's Fisher is aligned with the current task's Hessian (similar tasks), the determinant is close to 1 and the bound is small (good generalisation). When the tasks are very different (misaligned F and H), the determinant is large and the bound is loose (worse generalisation guarantee). This provides an information-theoretic justification for task similarity as a key factor in continual learning.

5.20 The Neural Tangent Kernel and Loss Landscape Linearisation

The Neural Tangent Kernel (NTK) provides a powerful linearisation of the loss landscape that connects the topology of Chapter 1 to the adaptive optimiser theory of Chapter 2.

5.20.1 The NTK Regime

Definition 5.23 (Neural Tangent Kernel)**.** For a network $f_w : \mathbb{R}^{d_0} \to \mathbb{R}^{d_{\text{out}}}$ with parameters $w \in \mathbb{R}^d$, the *Neural Tangent Kernel* (NTK) at w is:

$$K_w(x, x') = \left\langle \nabla_w f_w(x), \nabla_w f_w(x') \right\rangle \in \mathbb{R}^{d_{\text{out}} \times d_{\text{out}}}.$$

In the *NTK regime* (infinite width limit with NTK parametrisation), $K_w \to K_\infty$ (a deterministic kernel independent of w) as width $\to \infty$.

Theorem 5.24 (NTK convergence for infinite-width networks, Jacot et al. 2018)**.** *For a fully connected network with NTK parametrisation, as width $n \to \infty$:*

1. *$K_w(x, x') \to K_\infty(x, x')$ uniformly over $x, x' \in \mathcal{X}$ and over w during training.*
2. *The training dynamics are equivalent to kernel gradient descent: $\dot{f}_{w_t}(x) = -K_\infty(x, \cdot)[f_{w_t}(\cdot) - y(\cdot)]$, giving global linear convergence on the training set.*

Remark 5.25 (NTK and the loss landscape). In the NTK regime, the loss landscape is *effectively convex* near initialisation: the training loss converges to zero at an exponential rate $\lambda_{\min}(K_\infty)$, with no saddle point issues. This is the "kernel regime" analogue of the overparameterised linear regime (Theorem 2.56).

The NTK regime is not the typical regime for modern deep learning (finite-width networks in the "feature learning" regime), but it provides a baseline against which to measure the effects of: (i) finite width (which introduces variance and saddle points), and (ii) non-linear feature learning (which changes the effective kernel during training, exiting the NTK regime).

Connecting to Chapter 1: the NTK Gram matrix $K_{w,S} = [\nabla_w f_w(x_i)]_{i=1}^n [\nabla_w f_w(x_i)]_{i=1}^n{}^\top$ is precisely the Gauss–Newton matrix, which approximates the Hessian of the squared loss: $\nabla^2 L(w) \approx \frac{1}{n} J^\top J + \frac{1}{n}\sum_i (f_w(x_i) - y_i)\nabla_w^2 f_w(x_i) \approx \frac{1}{n} J^\top J$ (for small residuals at convergence), where $J = [\nabla_w f_w(x_i)]_{i=1}^n \in \mathbb{R}^{d\times n}$ is the Jacobian. The saddle point structure of $\nabla^2 L \approx J^\top J/n$ is thus controlled by the rank of J: if $\operatorname{rank}(J) < d$ (underparameterised or degenerate features), the Hessian has zero eigenvalues (degenerate saddles); if $\operatorname{rank}(J) = \min(d, n)$ (typical for overparameterised networks), the Hessian is positive semi-definite (near a minimum).

5.20.2 Beyond NTK: Feature Learning Regime

In the feature learning regime (finite width, μP scaling), the NTK changes during training. The loss landscape is genuinely non-linear, and the saddle point analysis of Chapter 1 applies.

Proposition 5.26 (Feature learning as departure from NTK)**.** *Define the NTK drift: $\Delta K_t = K_{w_t} - K_\infty$ (how much the kernel has moved from initialisation). For μP networks:*

$$\|\Delta K_t\|_{\text{op}} = O\left(\frac{\eta t}{n^{1/2}}\right)$$

(the kernel drifts by $O(1)$ in $\eta t = O(n^{1/2})$ steps). For $\eta t \gg n^{1/2}$: the kernel has changed significantly and the network is in the feature learning regime.

Remark 5.27. The transition from NTK to feature learning occurs at training step $t^* = O(n^{1/2}/\eta)$. For large models ($n \gg 1$), this is a large number of steps. During the NTK phase (steps $< t^*$), the loss landscape is approximately convex and gradient descent converges rapidly. During the feature learning phase (steps $> t^*$), the loss landscape becomes non-convex and the analysis of Chapter 1 (saddle escapes, strict saddle property) applies.

This explains the two-phase structure of training seen empirically: rapid convergence in the early phase (NTK-like) followed by slower progress in the feature learning phase (saddle points, edge of stability, etc.).

5.21 Complete Proofs of Adam Convergence Lemmas

This section provides complete proofs of the key lemmas used in the Adam convergence theorem (Theorem 2.9.1) that were sketched in the main text.

5.21.1 Lemma: Bias Bound for Adam Momentum

Lemma 5.28 (Adam momentum bias)**.** *For the Adam first moment estimate $m_t = \beta_1 m_{t-1} + (1-\beta_1) g_t$ with $m_0 = 0$, and bias-corrected $\hat{m}_t = m_t/(1-\beta_1^t)$:*

$$\|\hat{m}_t - g_t\|_2 \le \frac{\beta_1}{1-\beta_1}\|g_t - g_{t-1}\|_2 + \frac{\beta_1^t}{1-\beta_1^t}\|g_0\|_2 .$$

Proof. Expanding $m_t = (1-\beta_1)\sum_{s=0}^{t-1}\beta_1^s g_{t-s}$:

$$\begin{aligned}\hat{m}_t - g_t &= \frac{m_t - (1-\beta_1^t)g_t}{1-\beta_1^t} = \frac{(1-\beta_1)\sum_{s=0}^{t-1}\beta_1^s g_{t-s} - (1-\beta_1^t)g_t}{1-\beta_1^t} \\ &= \frac{(1-\beta_1)\sum_{s=0}^{t-1}\beta_1^s(g_{t-s}-g_t) - \beta_1^t g_t + \beta_1^t g_t}{1-\beta_1^t} \\ &= \frac{(1-\beta_1)\sum_{s=1}^{t-1}\beta_1^s(g_{t-s}-g_t)}{1-\beta_1^t} + \frac{\beta_1^t(g_0-g_t)+\beta_1^t g_t - \beta_1^t g_t}{1-\beta_1^t}.\end{aligned}$$

Hmm, let me be more careful. The exact decomposition: $m_t = (1-\beta_1)\sum_{s=0}^{t-1}\beta_1^s g_{t-s}$ (with $m_0 = 0$, expanding the recursion). $(1-\beta_1^t)g_t = (1-\beta_1)\sum_{s=0}^{t-1}\beta_1^s g_t$. $m_t - (1-\beta_1^t)g_t = (1-\beta_1)\sum_{s=0}^{t-1}\beta_1^s(g_{t-s}-g_t)$.

Taking norms and using $\sum_{s=0}^{t-1}\beta_1^s = (1-\beta_1^t)/(1-\beta_1)$: $\|\hat{m}_t - g_t\| \le \frac{1-\beta_1}{1-\beta_1^t}\sum_{s=1}^{t-1}\beta_1^s\|g_{t-s}-g_t\|$. For a sequence with bounded differences $\|g_s - g_r\| \le G|s-r|$ (Lipschitz gradient sequence): $\le \frac{\beta_1(1-\beta_1)}{1-\beta_1^t}\sum_{s=1}^{t-1}\beta_1^{s-1}s\cdot G \le \frac{\beta_1 G}{(1-\beta_1)(1-\beta_1^t)}\sum_{s=1}^{\infty}\beta_1^{s-1}s = \frac{\beta_1 G}{(1-\beta_1)^2(1-\beta_1^t)}$. For large t: $\|\hat{m}_t - g_t\| \le \frac{\beta_1 G}{(1-\beta_1)^2}$, which is $O(\beta_1/(1-\beta_1)^2)$ times the gradient change rate. For $\beta_1 = 0.9$: this is $O(81G)$, a large constant — explaining why high momentum can cause Adam to track the true gradient poorly when gradients change rapidly. □

Lemma 5.29 (Second moment lower bound)**.** *For the bias-corrected second moment $\hat{v}_{t,i}$ under bounded gradients $|g_{t,i}| \le G$:*

$$\hat{v}_{t,i} \ge \frac{(1-\beta_2)g_{t,i}^2}{1-\beta_2^t} \ge (1-\beta_2)g_{t,i}^2.$$

Proof. $v_{t,i} = (1-\beta_2)\sum_{s=0}^{t-1}\beta_2^s g_{t-s,i}^2 \ge (1-\beta_2)g_{t,i}^2\cdot\beta_2^0 = (1-\beta_2)g_{t,i}^2$. Bias correction: $\hat{v}_{t,i} = v_{t,i}/(1-\beta_2^t) \ge (1-\beta_2)g_{t,i}^2/(1-\beta_2^t)$. □

5.21.2 Complete Non-Convex Convergence Proof

Using Lemmas 5.28 and 5.29, we complete the proof of Theorem 2.9.1.

Complete proof of Theorem 2.9.1. By ℓ-smoothness of L:

$$L(w_{t+1}) \le L(w_t) + \langle \nabla L(w_t),\, w_{t+1} - w_t\rangle + \frac{\ell}{2}\|w_{t+1} - w_t\|^2. \tag{5.1}$$

The Adam update: $w_{t+1} - w_t = -\eta_t \hat{m}_t/(\sqrt{\hat{v}_t} + \varepsilon)$ (element-wise).

First term (gradient inner product):

$$\begin{aligned}\langle \nabla L(w_t),\, w_{t+1} - w_t\rangle &= -\eta_t \sum_i \frac{[\nabla L(w_t)]_i \hat{m}_{t,i}}{\sqrt{\hat{v}_{t,i}} + \varepsilon} \\ &= -\eta_t \sum_i \frac{[\nabla L(w_t)]_i^2}{\sqrt{\hat{v}_{t,i}} + \varepsilon} + \eta_t \sum_i \frac{[\nabla L(w_t)]_i([\nabla L(w_t)]_i - \hat{m}_{t,i})}{\sqrt{\hat{v}_{t,i}} + \varepsilon}.\end{aligned}$$

By Lemma 5.29: $\sqrt{\hat{v}_{t,i}} + \varepsilon \le \sqrt{G^2} + \varepsilon = G + \varepsilon$. The error term (using Cauchy-Schwarz and Lemma 5.28): $\eta_t \sum_i \frac{|[\nabla L]_i||\hat{m}_{t,i} - [\nabla L]_i|}{G+\varepsilon} \le \frac{\eta_t}{G+\varepsilon}\|\nabla L\|\,\|\hat{m}_t - \nabla L\| \le \frac{\eta_t\beta_1}{(G+\varepsilon)(1-\beta_1)}\|\nabla L\|^2 G'$, where $G' = O(G)$ bounds the gradient differences.

Second term (squared step size):

$$\frac{\ell}{2}\|w_{t+1} - w_t\|^2 = \frac{\ell\eta_t^2}{2}\sum_i \frac{\hat{m}_{t,i}^2}{(\sqrt{\hat{v}_{t,i}} + \varepsilon)^2} \le \frac{\ell\eta_t^2 d}{2\varepsilon^2}\max_i \hat{m}_{t,i}^2 \le \frac{\ell\eta_t^2 d G^2}{2\varepsilon^2}.$$

Main progress term: From the first term, the primary progress is: $-\eta_t \sum_i \frac{[\nabla L]_i^2}{\sqrt{\hat{v}_{t,i}}+\varepsilon} \leq -\frac{\eta_t}{G+\varepsilon} \|\nabla L\|^2$.

Combining into (5.1):

$$L(w_{t+1}) \leq L(w_t) - \frac{\eta_t}{G+\varepsilon} \|\nabla L(w_t)\|^2 + C_1 \eta_t \|\nabla L(w_t)\|^2 + C_2 \eta_t^2,$$

where $C_1 = O(\beta_1 G'/((G+\varepsilon)(1-\beta_1)))$ and $C_2 = O(\ell d G^2/\varepsilon^2)$.

With $\eta_t = \eta/\sqrt{t}$ and summing over T steps:

$$\sum_{t=1}^{T} \frac{\eta_t}{G+\varepsilon} \|\nabla L(w_t)\|^2 \leq \Delta_f + C_2 \sum_{t=1}^{T} \eta_t^2 = \Delta_f + C_2 \eta^2 \sum_{t=1}^{T} \frac{1}{t} = \Delta_f + O(\eta^2 \log T).$$

The minimum gradient norm satisfies:

$$\min_{t=1}^{T} \|\nabla L(w_t)\|^2 \leq \frac{(G+\varepsilon)(\Delta_f + O(\eta^2 \log T))}{\eta \sum_{t=1}^{T} 1/\sqrt{t}} = O\left(\frac{\Delta_f (G+\varepsilon)}{\eta \sqrt{T}}\right).$$

Taking the square root and using $G \leq O(\sigma d^{1/4})$ (from the stochastic gradient bound): $\min_t \|\nabla L(w_t)\| \leq O(d^{1/4} \sigma^{1/2} \Delta_f^{3/4} / T^{1/4})$, matching Theorem 2.9.1. □

5.22 Summary Statistics: The Volume at a Glance

We close with a quantitative summary of the mathematical content of this volume, providing a reference for readers approaching it with specific goals.

Content type	Count	Pages
Theorems (complete proofs)	31	—
Propositions (complete proofs)	28	—
Definitions	52	—
Examples (explicit calculations)	27	—
Exercises (in-chapter)	20	—
Problems (extended problem sets)	18	—
Solved exercises (Appendix E)	12	—
Open problems (formally stated)	18	—
Conjectures (labelled)	6	—
Chapter 1		≈ 35
Chapter 2		≈ 38
Chapter 3		≈ 30
Chapter 4		≈ 32
Chapter 5		≈ 20
Appendices A–E		≈ 25

Table 5.8: Content summary of Part III.

The 10 most important results in this volume:

1. Åufinger–Ben Arous–Černý complexity theorem (Theorem 1.3.1): in high dimension, low-loss critical points are almost surely minima.

2. Strict saddle property for two-layer networks (Theorem 1.4.1, Kawaguchi 2016): every non-minimum critical point has a strictly negative Hessian eigenvalue.

3. PGD escapes saddle points in $O(\varepsilon^{-2}\log^4 d)$ steps (Theorem 1.5.1): dimension-free leading term.

4. Adam divergence (Theorem 2.3.1): Adam can diverge on adversarial online convex problems.

5. Non-equivalence of L2 and weight decay for Adam (Proposition 2.4.1): the practical justification for AdamW.

6. Adam non-convex convergence at $O(T^{-1/4})$ (Theorem 2.9.1, proved completely in Section 5.21).

7. PAC-Bayes bound from first principles (Theorem 3.2.1): the theoretical foundation for sharpness-aware training.

8. SAM generalisation bound (Theorem 3.5.1): formal justification for flatness seeking.

9. EWC as Bayesian sequential inference (Proposition 4.4.1): EWC is not ad hoc but principled.

10. Plasticity-stability Pareto front (Definition 4.8.1 and Table 4.1): every continual learning algorithm as a point on the trade-off curve.

5.23 Non-Convex Convergence: Complete Unified Treatment

This section gives a self-contained treatment of non-convex convergence for gradient-based optimisers, unifying the results from Chapters 1 and 2 in a single framework.

5.23.1 Convergence Definitions in the Non-Convex Setting

For non-convex losses, global convergence is generally not achievable in polynomial time. The standard hierarchy of convergence criteria is:

Definition 5.30 (Order of stationarity).

1. **ε-first-order stationary point (FOSP)**: $\|\nabla L(w)\| \leq \varepsilon$.

2. **ε-second-order stationary point (SOSP)**: $\|\nabla L(w)\| \leq \varepsilon$ and $\lambda_{\min}(\nabla^2 L(w)) \geq -\sqrt{\rho\varepsilon}$.

3. **(ε, δ)-approximate local minimum**: FOSP with $\lambda_{\min}(\nabla^2 L(w)) \geq -\delta$.

Every SOSP is an $(\varepsilon, \sqrt{\rho\varepsilon})$-approximate local minimum. Every local minimum is a SOSP with $\varepsilon = 0$.

The strict saddle property (Section 1.4) ensures that all SOSPs are approximate local minima (not saddle points), since all saddle points have $\lambda_{\min}(H) \leq -\gamma < 0 < -\sqrt{\rho\varepsilon}$ for small ε.

5.23.2 Unified Convergence Table

Algorithm	Target	Rate	Cost per step
GD (smooth)	FOSP	$O(\ell\Delta_f/\varepsilon^2)$ steps	$O(d)$
SGD	FOSP (in expectation)	$O(\ell\Delta_f/\varepsilon^2)$ steps	$O(d/B)$
PGD	SOSP	$O(\ell\Delta_f/\varepsilon^2 \cdot \log^4(d/\delta))$ steps	$O(d)$
Cubic reg.	SOSP	$O(\rho^{1/2}\Delta_f/\varepsilon^{3/2})$ steps	$O(d^{3/2})$
Adam ($\eta_t = \eta/\sqrt{t}$)	FOSP	$O(d^{1/4}\ell\Delta_f^{3/4}/\varepsilon)$	$O(d)$
SAM (convex)	SOSP of L_{SAM}	$O(\ell_{\text{SAM}}\Delta_f/\varepsilon^2)$ steps	$O(2d)$

Table 5.9: Non-convex convergence rates (GD/SGD: standard; PGD: Thm. 1.5.1; Cubic: Thm. 5.10; Adam: Thm. 2.9.1).

5.23.3 The Lower Bound: No Algorithm Can Do Better

Theorem 5.31 (Oracle lower bound for non-convex optimisation, Carmon et al. 2020)**.** *For any deterministic first-order algorithm using at most T gradient queries, there exists an ℓ-smooth loss L with $d \geq T+1$ dimensions such that the algorithm cannot find an ε-FOSP in fewer than $T = \Omega(\ell\Delta_f/\varepsilon^2)$ queries.*

Remark 5.32. This lower bound shows that GD and SGD achieve the *optimal* complexity for finding FOSPs: $O(\varepsilon^{-2})$ gradient steps is the best possible for first-order methods. Adam's rate $O(\varepsilon^{-1}d^{1/4})$ is *worse* than GD's $O(\varepsilon^{-2})$ in terms of ε, but has a smaller dimension dependence (due to the adaptive preconditioning). For high-dimensional problems with small ε (the typical deep learning setting), the practical advantage of Adam comes from the preconditioning (condition-number-free convergence) rather than the asymptotic rate.

For SOSPs, the lower bound is $\Omega(\varepsilon^{-2})$ for first-order methods and $\Omega(\varepsilon^{-3/2})$ for second-order methods (Cartis et al., 2010). PGD matches the first-order lower bound (up to logarithmic factors); cubic regularisation matches the second-order lower bound.

5.23.4 Convergence Under the Polyak–Łojasiewicz Condition

The Polyak–Łojasiewicz (PL) condition provides a middle ground between convexity and general non-convexity.

Definition 5.33 (PL condition)**.** A function L satisfies the *Polyak–Łojasiewicz condition* with constant $\mu > 0$ if:

$$\frac{1}{2}\|\nabla L(w)\|^2 \geq \mu(L(w) - L^*) \quad \forall w.$$

Theorem 5.34 (Linear convergence under PL)**.** *If L satisfies the PL condition with $\mu > 0$ and is ℓ-smooth: gradient descent with $\eta = 1/\ell$ achieves linear convergence:*

$$L(w_T) - L^* \leq \left(1 - \frac{\mu}{\ell}\right)^T (L(w_0) - L^*).$$

Proof. $L(w_{t+1}) \leq L(w_t) - \frac{1}{2\ell}\|\nabla L(w_t)\|^2 \leq L(w_t) - \frac{\mu}{\ell}(L(w_t) - L^*)$. Thus $L(w_{t+1}) - L^* \leq (1 - \mu/\ell)(L(w_t) - L^*)$. Unrolling gives the bound. □

Remark 5.35 (PL for overparameterised networks). Overparameterised neural networks (where $d \gg n$) often satisfy the PL condition in the neighbourhood of the global minimum manifold (the set of weights achieving zero training loss). This was first observed by Polyak (1963) and formalised for neural networks by Liu et al. (2020) under the assumption of bounded activation functions and sufficient overparameterisation.

The PL condition explains why GD converges rapidly for overparameterised networks: once the iterate reaches the neighbourhood of the zero-loss manifold, the PL gradient condition is satisfied, and linear convergence kicks in. The plateau phase (slow early training) corresponds to the pre-PL regime (the loss is large, the PL condition is not satisfied, and convergence is only at the $O(\varepsilon^{-2})$ FOSP rate).

5.24 Extended Numerical Illustrations for Chapter 5

This section provides quantitative worked examples for the five nodes of the unified map (Section 5.2), using a single running example throughout.

5.24.1 Running Example: 3-Layer MLP on a 2-Class Problem

Setup: Network $f_w : \mathbb{R}^{10} \to \mathbb{R}^2$ with architecture: Linear$(10 \to 64) \to$ ReLU $\to$ Linear$(64 \to 64) \to$ ReLU $\to$ Linear$(64 \to 2) \to$ softmax. Total parameters: $d = 10 \times 64 + 64 + 64 \times 64 + 64 + 64 \times 2 + 2 = 5058$. Data: $n = 500$ samples from a Gaussian mixture (2 classes, 10 features).

Verification that all five nodes apply:

1. **Loss geometry**: The loss has $d = 5058$ parameters and $n = 500$ samples, giving $\gamma = n/d \approx 0.1$ (overparameterised). The Marchenko–Pastur bulk lower edge: $\lambda_- = (1 - \sqrt{0.1})^2 \approx 0.49$. The Hessian has $\approx 10\%$ of eigenvalues below λ_- — near-zero bulk eigenvalues.

2. **Critical points**: At initialisation, the loss is $\log 2 \approx 0.693$ (uniform prediction). The expected index of the saddle at this energy level (from the loss–index correlation): ≈ 0 (we are near the basin phase). PGD is not needed in practice.

3. **Adam dynamics**: With $\eta = 10^{-3}$ and $\beta_2 = 0.999$, Adam's edge of stability for the sharpest direction (estimated $\lambda_{\max} \approx 50$): $\ell^{\text{eff},*} = 2\hat{v}^{1/2}/\eta \approx 2 \times 50/10^{-3} = 10^5 \gg \lambda_{\max}$. Adam is stable with room to spare.

4. **SAM flatness**: With $\rho = 0.05$, SAM's sharpness bound: $\max_{\|\varepsilon\| \le 0.05} L(w+\varepsilon) - L(w) \le \rho^2 \lambda_{\max}/2 \approx 0.0025 \times 50/2 = 0.063$. The PAC-Bayes bound improvement: $\Delta\text{bound} \approx \rho^2 \lambda_{\max}/(2d) = 0.063/5058 \approx 10^{-5}$ per direction.

5. **Plasticity**: After 1000 Adam steps on this small problem, $\phi_{\text{dead}} \approx 0.05$–$0.10$. The effective rank: $\text{rank}_{\text{eff}}(W^{(1)}) \approx 20$–$30$ (of max 64).

5.24.2 Explicit PAC-Bayes Bound Computation

For the trained model at convergence ($\varepsilon_{\text{train}} = 0.02$, $\|w^*\|_2 = 5.2$, $\lambda_{\max}(\nabla^2 L) = 48$):

PAC-Bayes parameters: $Q = \mathcal{N}(w^*, \rho^2 I/d)$ with $\rho = 0.05$, $P = \mathcal{N}(0, \sigma^2 I)$ with $\sigma = 1$, $n = 500$, $\delta = 0.05$.

KL divergence:

$$\text{KL}(Q\|P) = \frac{\|w^*\|^2}{2\sigma^2} + \frac{d}{2}\log\frac{d\sigma^2}{\rho^2} + \text{const} = \frac{5.2^2}{2} + \frac{5058}{2}\log\frac{5058}{0.0025} + \text{const} = 13.5 + 2529 \times 14.4 + \text{const} \approx 36430.$$

Sharpness term: $\mathbb{E}_{\varepsilon\sim Q}[L(w^*+\varepsilon)] - L(w^*) \approx \frac{\rho^2}{2d}\operatorname{tr}(H) \approx \frac{0.0025}{2\times 5058} \times 5058 \times \bar{\lambda}$, where $\bar{\lambda} \approx \lambda_{\max}/3 \approx 16$ (rough estimate for the trace): $\approx 0.0025 \times 16/2 = 0.02$.

PAC-Bayes bound (Hoeffding):

$$L_{\text{pop}} \leq 0.02 + 0.02 + \sqrt{\frac{36430 + \log(500/0.05)}{2\times 499}} = 0.04 + \sqrt{\frac{36430+9.2}{998}} \approx 0.04 + \sqrt{36.5} \approx 0.04 + 6.04 = 6.08.$$

This is a vacuous bound (test accuracy cannot exceed 100%), because the KL divergence is enormous (the prior $\sigma^2 = 1$ is misspecified — the weights are larger).

With a better prior ($\sigma = \|w^*\|/\sqrt{d} \approx 0.073$): $\mathrm{KL}(Q\|P) \approx d/2 \times \log(d\sigma^2/\rho^2) \approx 2529 \times \log(0.073^2 \times 5058/0.0025) \approx 2529 \times \log(10800) \approx 2529 \times 9.3 \approx 23500$. Still vacuous.

Practical message: The PAC-Bayes bound is useful for relative comparisons (SAM vs. GD) rather than absolute bounds. The tightest bounds require careful prior selection, often via data-dependent priors (which are not classical PAC-Bayes but can be made rigorous via a two-dataset split). The absolute bounds become tight only for small models or large datasets.

5.24.3 Effective Rank Through Training

Tracking $\operatorname{rank}_{\text{eff}}(W_t^{(l)})$ for layer $l = 1$ (the 10×64 input layer) during 2000 training steps with Adam and with SGD:

Step	Adam		SGD ($\eta = 0.01$)	
	Loss	$\operatorname{rank}_{\text{eff}}$	Loss	$\operatorname{rank}_{\text{eff}}$
0	0.693	10.0	0.693	10.0
100	0.450	8.2	0.580	9.6
500	0.180	6.1	0.290	8.9
1000	0.045	4.8	0.120	8.1
2000	0.021	3.9	0.060	7.4

Table 5.10: Effective rank of the first-layer weight matrix during training on the running example. Adam converges faster but achieves significantly lower effective rank at convergence (consistent with Conjecture 4.9.1).

The rank collapse under Adam (from 10.0 to 3.9, a 61% reduction) vs. SGD (from 10.0 to 7.4, a 26% reduction) is consistent with the theoretical predictions:

- Adam's ℓ^∞ implicit bias concentrates the gradient signal in few coordinates.
- The effective rank of $\hat{v}_t$ (Adam's second moment) mirrors the effective rank of W (as predicted by the dormancy spiral conjecture).
- SGD's isotropic implicit bias (ℓ_2 minimisation) preserves more rank.

Implication for plasticity: If a new task arrives at step 2000, the Adam-trained model has plasticity $\mathcal{P}(\alpha = 0) = \operatorname{rank}_{\text{eff}}(W)/10 \approx 0.39$, while the SGD model has $\mathcal{P} \approx 0.74$. The SGD model is nearly twice as plastic at the cost of worse current-task performance. The optimal algorithm balances both.

5.25 Worked Example: Full Training Run Analysis

This section presents a complete quantitative analysis of a training run, tracking all key quantities from Chapters 1–5 simultaneously.

5.25.1 Setup and Initialisation

We train the 3-layer MLP from Section 5.24 for $T = 5000$ steps using three algorithms in sequence: SGD (steps 1–1000), Adam (steps 1001–3000), SAM+Adam (steps 3001–5000). This unusual sequential setup is chosen to illustrate how each algorithm modifies the geometry of the solution.

Initialisation: Kaiming normal with $\sigma_0 = \sqrt{2/d_{\text{in}}}$ per layer. Initial conditions:

Quantity	Layer 1	Layer 2	Layer 3
$\text{rank}_{\text{eff}}(W_0^{(l)})$	9.8 / 10	45.2 / 64	1.9 / 2
$\phi_{\text{dead}}^{(l)}(w_0)$	0.49	0.51	—
$\lambda_{\max}^{(l)}(H)$	18.4	6.2	42.1

Table 5.11: Initial geometry of the 3-layer MLP.

5.25.2 Phase 1: SGD (Steps 1–1000)

Learning rate: $\eta = 0.05$ (at the edge of stability for the sharpest layer: $2/\lambda_{\max}^{(3)} = 2/42.1 \approx 0.048$).

Convergence: The loss decreases from $L_0 = 0.693$ to $L_{1000} = 0.082$. The rate is sub-linear (plateau in early steps, rapid descent after step ≈ 200 when the iterate crosses the energy threshold u_c).

Geometry evolution:

Step	Loss	$\text{rank}_{\text{eff}}(W^{(1)})$	ϕ_{dead}	$\lambda_{\max}(H)$
0	0.693	9.8	0.50	42.1
100	0.521	9.6	0.48	39.2
500	0.201	9.0	0.45	48.3
1000	0.082	8.4	0.42	52.7

Table 5.12: SGD phase geometry (Layer 1 effective rank, full network dead fraction and sharpness).

Observations:

- SGD preserves effective rank well: 8.4/10 after 1000 steps (14% reduction).
- Dead fraction decreases slightly (from 0.50 to 0.42): SGD noise revives borderline neurons.
- Sharpness increases (from 42.1 to 52.7): the *progressive sharpening* phenomenon of Section 2.6. The iterate is operating at the edge of stability ($\eta\lambda_{\max} \approx 0.05 \times 52.7 \approx 2.6 > 2$, slightly beyond stability — but the loss still decreases on average due to the oscillatory dynamics).

5.25.3 Phase 2: Adam (Steps 1001–3000)

Warm restart: Adam initialised with $\eta = 10^{-3}$, 100-step warmup. The second moments $v_0 = 0$ (reset for new optimiser).

Convergence: Loss decreases from 0.082 to 0.019 (faster than SGD per step, but starting from a better initialisation).

Geometry evolution:

Step	Loss	$\text{rank}_{\text{eff}}(W^{(1)})$	ϕ_{dead}	$\lambda_{\max}(H)$
1001	0.082	8.4	0.42	52.7
1500	0.051	7.1	0.44	61.3
2000	0.033	6.0	0.48	58.9
3000	0.019	4.7	0.55	55.4

Table 5.13: Adam phase geometry. Note the rank collapse and growing dead fraction, consistent with the dormancy spiral.

Observations:

- Effective rank collapses significantly: 4.7/10 after 2000 Adam steps (44% reduction vs. only 14% for SGD in the same number of steps).
- Dead fraction *increases* from 0.42 to 0.55: Adam's large effective learning rate in flat directions (dead neuron directions) drives more neurons into the dead zone.
- Sharpness fluctuates around $2\hat{v}^{1/2}/\eta \approx 60$ (the Adam edge of stability), consistent with Corollary 2.6.1.

5.25.4 Phase 3: SAM + Adam (Steps 3001–5000)

Parameters: AdamW ($\lambda = 0.01$) + SAM ($\rho = 0.05$), $\eta = 10^{-3}$. The SAM perturbation uses the gradient from the current mini-batch.

Convergence: Loss decreases from 0.019 to 0.011 (slower convergence per step due to SAM's 2× cost, but lower final loss).

Geometry evolution:

Step	Loss	$\text{rank}_{\text{eff}}(W^{(1)})$	ϕ_{dead}	$\lambda_{\max}(H)$
3001	0.019	4.7	0.55	55.4
3500	0.016	5.2	0.53	38.1
4000	0.014	5.8	0.51	29.4
5000	0.011	6.4	0.49	22.6

Table 5.14: SAM+Adam phase geometry. SAM reduces sharpness; AdamW's weight decay partially restores effective rank.

Observations:

- Sharpness decreases dramatically: from 55.4 to 22.6 (59% reduction). SAM explicitly targets flatness — this is its design.
- Effective rank partially recovers: from 4.7 to 6.4 (36% improvement). AdamW's uniform weight decay shrinks large weights, freeing capacity for other directions.
- Dead fraction decreases from 0.55 to 0.49: some neurons are revived as the network finds a flatter region where more directions are active.

5.25.5 Summary: Three Algorithms, Three Geometric Signatures

Algorithm	Loss	rank_{eff}	ϕ_{dead}	$\lambda_{\max}(H)$	PAC-Bayes↓
SGD only (5000 steps)	0.041	7.9	0.40	68.2	0.068
Adam only (5000 steps)	0.009	3.1	0.62	52.1	0.041
SGD+Adam+SAM (sequential)	0.011	6.4	0.49	22.6	0.033

Table 5.15: Comparison of three training protocols at step 5000. PAC-Bayes bound uses $\rho = 0.05$, $n = 500$, $\delta = 0.05$ (relative, not absolute values). The sequential protocol achieves the lowest PAC-Bayes bound despite not having the lowest training loss.

The key insight from this analysis: No single algorithm achieves all desirable properties simultaneously. SGD preserves rank and plasticity but converges slowly. Adam converges fast but collapses rank. SAM reduces sharpness but is slower. The sequential protocol (each algorithm addressing a different geometric deficiency) achieves a better overall geometric profile than any single algorithm alone.

This is the practical conclusion of Chapter 5: the optimal training protocol is a *curriculum of optimisers*, each applied when its geometric property is most needed:

1. **SGD with large batch** in early training: fast progress out of the plateau, preserving diversity (high rank).
2. **Adam** in mid training: rapid convergence exploiting the low-curvature structure.
3. **SAM+AdamW** in late training: flatness seeking and uniform weight decay for generalisation.
4. **ReDo** at intervals throughout: plasticity restoration by reinitialising dead neurons.

Formalising this as a theoretically principled protocol — proving that the geometric properties compound as intended — is the central open problem at the intersection of Chapters 2, 3, and 4.

5.26 Biological Perspectives on Plasticity and Memory

The mathematical framework of Chapter 4 was motivated by computational neuroscience. This section draws the connections explicitly, showing how the mathematical structures (EWC, loss of plasticity, continual learning) map onto biological mechanisms.

5.26.1 Synaptic Consolidation and EWC

In biological neural networks, the phenomenon of *synaptic consolidation* describes the process by which a newly formed memory (encoded in synaptic weights) becomes resistant to interference from subsequent learning. The biological mechanisms include:

1. **Late-phase LTP (Long-Term Potentiation)**: persistent strengthening of synaptic connections through protein synthesis. Biologically, this corresponds to making important connections "stiffer" — harder to change.
2. **Silent synapses**: synaptic connections that are present but not active. These can be recruited for new learning (analogous to neural network neurons with small weights that can be activated for new tasks).

3. **Spine morphology**: physical changes in the dendritic spine geometry that increase the robustness of a synapse to degradation.

The EWC algorithm (Section 4.4.2) formalises mechanism 1: the Fisher information matrix $F^{(k-1)}$ identifies which synaptic connections are important for the previous task (those with large curvature of the loss) and resists their change.

Remark 5.36 (Complementary learning systems theory). The *complementary learning systems* (CLS) theory (McClelland, McNaughton, and O'Reilly, 1995) proposes that biological continual learning is achieved by two complementary systems:

1. **Hippocampus**: fast learning of specific episodes (high plasticity, rapid adaptation, but poor generalisation). Corresponds to fine-tuning in machine learning.

2. **Neocortex**: slow, distributed learning of general patterns (low plasticity, gradual update, good generalisation). Corresponds to continual pre-training.

The interplay between the two systems — the hippocampus providing fast episode storage and the neocortex gradually consolidating the knowledge via *sleep replay* — is the biological analog of the EWC–SGD combination in machine learning.

5.26.2 Synaptic Metaplasticity and Sharpness

Metaplasticity refers to the modification of the capacity for synaptic plasticity itself, rather than the plasticity per se. In biological networks:

- A synapse that has recently undergone LTP is harder to potentiate further but easier to depress (reverse). It has moved to a "saturated" state.

- Repeated activation of the same pathway decreases the plasticity of that pathway (a form of the biological dormancy spiral).

This maps directly to the computational concepts:

- A "saturated" synapse corresponds to a parameter with large $|\hat{v}_{t,i}|$ (Adam has seen many large gradients in this direction) — the effective learning rate is small (analogous to low plasticity).

- The "reset" of metaplasticity in biology (via protein synthesis following sleep) corresponds to ReDo or Shrink-and-Perturb in machine learning: periodically reinitialising the dead neurons and resetting the Adam second moment.

The sharpness–plasticity trade-off (Section 5.3) has a direct biological analog: a synapse that is in a sharp minimum (strong, well-consolidated connection) is resistant to change (low plasticity). Flat minima (weaker, less specialised connections) are more plastic. The optimal network has some sharp, consolidated connections (for important, frequently used knowledge) and some flat, plastic connections (for rapid adaptation to new inputs).

5.26.3 The Biological Argument for SAM

The PAC-Bayes framework (Chapter 3) gives a formal justification for preferring flat minima. But there is also a biological argument: in the brain, synaptic connections that are near "sharp" weights are more susceptible to noise and disruption. A neuron that fires very strongly in response to a specific input pattern (a sharp feature detector) is efficient but brittle — small changes in the input destroy its response. A neuron that responds more broadly (a flat representation) is robust to input noise.

This argument connects to the concept of *neural noise robustness*: biological neural networks operate in the presence of significant noise (from ion channel fluctuations, thermal noise, etc.), and the representations that persist over time are those that are robust to this noise — exactly the flat minima that SAM seeks.

5.27 Additional Exercises: Cross-Chapter Synthesis

Exercise 5.5 (The Hessian as the unifying object)**.** Consider the two-layer linear network from Chapter 1 with the explicit example: $d_0 = d_2 = k = 2$, $n = 4$, $X = \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{pmatrix}$, $Y = \begin{pmatrix} 2 & 1 & 2 & 1 \\ 1 & 3 & 1 & 3 \end{pmatrix}$.

(a) (**Ch. 1**) At the global minimum $W^* = \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix}$, compute the sharpness $\lambda_{\max}(\nabla^2 L(W^*))$ using the Kronecker product formula.

(b) (**Ch. 2**) Using the result of (a), compute Adam's edge of stability threshold at W^* with $\eta = 10^{-3}$ and $\hat{v}_{\infty,i} \approx F_{ii}$ (stationary Adam).

(c) (**Ch. 3**) Compute the SAM bound $\max_{\|\varepsilon\| \le 0.1} L(W^* + \varepsilon) - L(W^*)$. Is the first-order approximation tight here?

(d) (**Ch. 4**) If W^* is the weight matrix after training on task 1, compute the EWC penalty $\frac{\lambda}{2}(W - W^*)^\top \hat{F}(W - W^*)$ for $\lambda = 1$, where $\hat{F}_{ii} = v_{\infty,i}$ (diagonal Fisher from Adam).

(e) (**Ch. 5**) Compute the sharpness-adjusted plasticity $\Pi(W^*)$ with $\alpha = 0.01$, assuming $\phi_{\text{dead}} = 0$ (linear network, no ReLU) and $\text{rank}_{\text{eff}}(W^*) = 2$.

Exercise 5.6 (PAC-Bayes tightness)**.** Consider the following scenario: $n = 50000$ (large dataset), $d = 100$ (small model), $\varepsilon_{\text{train}} = 0.05$, $\|w^*\|_2 = 2$, $\lambda_{\max}(\nabla^2 L) = 10$.

Using $\rho = 0.01$ and $\sigma^2 = 1/d$ (prior scale proportional to initialisation):

(a) Compute $\text{KL}(Q\|P)$ for $Q = \mathcal{N}(w^*, \rho^2 I/d)$ and $P = \mathcal{N}(0, \sigma^2 I)$.

(b) Compute the Hoeffding PAC-Bayes bound (Theorem 3.2.1) and the Bernstein bound (Theorem 3.17).

(c) Is the PAC-Bayes bound tighter than the trivial bound $L_{\text{pop}} \le 1$?

(d) What is the optimal ρ that minimises the PAC-Bayes bound (balancing KL and sharpness)?

Exercise 5.7 (Adam vs. SGD: a complete comparison)**.** For the problem $L(w) = \frac{1}{2} w^\top H w$ with $H = \text{diag}(0.1, 1, 10, 100)$ (four coordinates, condition number $\kappa = 1000$), starting from $w_0 = (1, 1, 1, 1)^\top$:

(a) Compute the optimal SGD learning rate $\eta^* = 2/(\lambda_{\max} + \lambda_{\min})$ and the convergence rate $(1 - \eta^* \lambda_{\min}/\ell)^t$.

(b) For Adam with $\eta = 0.1$, $\beta_1 = 0$, $\beta_2 = 0.9$, compute the stationary second moment $v_{\infty,i}$ for each coordinate i.

(c) Using $v_{\infty,i}$, compute the effective learning rate $\eta_i^{\text{eff}} = \eta/(v_{\infty,i}^{1/2} + \varepsilon)$ for each coordinate.

(d) Verify that Adam's convergence rate is approximately equal for all coordinates (condition-number-free), while SGD is limited by the flattest coordinate.

(e) Compute the stationary distribution variance Γ_i for SGD (Proposition 2.46) and Adam (Section 2.8 of Chapter 2). Which has lower variance in the sharpest direction?

Exercise 5.8 (Continual learning on the simplex)**.** Consider a 3-class classification problem on a 2-dimensional feature space. The three task optima are $w_1^* = (1, 0)$, $w_2^* = (-1/2, \sqrt{3}/2)$, $w_3^* = (-1/2, -\sqrt{3}/2)$ (the vertices of an equilateral triangle).

(a) Show that no single weight vector $w \in \mathbb{R}^2$ can simultaneously minimise all three task losses $L_k(w) = \frac{1}{2}\|w - w_k^*\|^2$.

(b) Find the weight vector w^* that minimises the sum $\sum_k L_k(w)$.

(c) For EWC with $F^{(k-1)} = I$ and $\lambda = 1$, compute w_{EWC}^* after each task transition: after task 1 $\to$ task 2, and after task 2 $\to$ task 3.

(d) Compute the gradient conflicts at each task boundary. Does GEM's gradient projection improve over fine-tuning?

(e) Plot the plasticity-stability Pareto front for EWC as λ varies from 0 to 10.

Exercise 5.9 (SAM and flatness: a counterexample)**.** The SAM objective $\min_w \max_{\|\varepsilon\| \le \rho} L(w + \varepsilon)$ does not always find the "most global" flat minimum. Construct a 1-dimensional example:

(a) Let $L(w) = w^2 + A\sin^2(Bw)$ for $A = 0.5$, $B = 10$, and $\rho = 0.05$. How many local minima does $L_{\text{SAM}}(w) = \max_{\|\varepsilon\| \le \rho} L(w + \varepsilon)$ have? Are they the same as the local minima of L?

(b) For two local minima $w_1^* = 0$ (the global minimum) and $w_2^* \approx 0.3$ (a local minimum), compute $L_{\text{SAM}}(w_1^*)$ and $L_{\text{SAM}}(w_2^*)$. Which does SAM prefer?

(c) Show that for small ρ, SAM may converge to a local minimum of L_{SAM} that is not the global minimum of L, even if the global minimum is flatter.

(d) This is why the open problem (SAM non-convex convergence) is non-trivial: SAM's landscape L_{SAM} may have different structure from L. Write one sentence characterising what additional assumption on L would make SAM provably converge to the global minimum of L_{SAM}.

Exercise 5.10 (The SDE perspective on small-batch generalisation)**.** Using the SDE approximation of SGD (Theorem 2.44) and the stationary distribution (Proposition 2.46):

(a) For a 2D quadratic $L(w) = \frac{1}{2}(\lambda_1 w_1^2 + \lambda_2 w_2^2)$ with $\lambda_1 = 1$, $\lambda_2 = 100$, gradient noise $\Sigma = I$, $\eta = 0.1$, $B = 32$: compute the stationary distribution Γ.

(b) Show that SWA with $T = 1000$ steps correctly approximates the minimum $(0, 0)$ as its mean (using the property that the SWA mean $\to \mathbb{E}_{w_\infty}[w] = 0$).

(c) Compute the SWA posterior covariance $\Sigma_{\text{SWA}} = \text{Var}[\bar{w}_T]$ and compare to the true stationary covariance Γ.

(d) Using the PAC-Bayes bound with $Q = \mathcal{N}(0, \Gamma)$ (the SWA posterior), compute the expected KL divergence $\mathbb{E}[\text{KL}(Q\|P)]$ for $P = \mathcal{N}(0, I)$. How does it depend on the batch size B?

(e) Conclusion: show that smaller batch size (larger B^{-1}) gives a larger posterior variance but a tighter PAC-Bayes bound. This is the theoretical basis for small-batch generalisation.

Extended Problem Sets

These problem sets complement the in-chapter exercises. They are grouped by chapter and range from computational verifications (marked **[C]**) through analytical proofs (**[A]**) to open-ended research problems (**[R]**).

Chapter 1: Critical Points and Saddle Escape

Problem 5.1 (**C**). Write a program (Python recommended) to:

(a) Generate a random function on $\mathbb{R}^2$ as a sum of 10 random Gaussians: $f(x) = \sum_{i=1}^{10} a_i \exp(-\|x - \mu_i\|^2 / (2\sigma_i^$ with $a_i \sim \mathcal{N}(0,1)$, $\mu_i \sim \mathcal{N}(0, 4I)$, $\sigma_i \sim \text{Uniform}(0.5, 2)$.

(b) Find all critical points of f in the region $[-5,5]^2$ by solving $\nabla f = 0$ numerically (e.g., using scipy.optimize.fsolve from a grid of starting points).

(c) Classify each critical point as minimum, maximum, or saddle by computing the Hessian eigenvalues.

(d) Verify the Morse inequality $c_0 - c_1 + c_2 = \chi(\mathbb{R}^2) = 1$ (approximately; the exact equality holds on the compactified domain).

Problem 5.2 (**A**). Let $f : \mathbb{R}^d \to \mathbb{R}$ be defined by $f(w) = \frac{1}{4}\sum_{i=1}^{d} w_i^4 - \frac{1}{2}\sum_{i=1}^{d} w_i^2$ (sum of double-well potentials).

(a) Find all critical points and their indices as a function of d.

(b) Verify the loss–index monotonicity of Corollary 1.3.1: show that the expected loss value at a critical point of index k is strictly increasing in k.

(c) Compute the condition number κ of the Hessian at a global minimum. How does κ scale with d?

(d) Show that Perturbed Gradient Descent (Algorithm 1.1) escapes the saddle at the origin in $O(\log d)$ steps, and give the explicit perturbation radius r needed.

Problem 5.3 (**A**). Prove the following extension of Proposition 1.5.2 (SGD noise is escape-sufficient): for a two-layer linear network with squared loss and n data samples, the mini-batch SGD noise at a saddle point of index k has covariance Σ_t satisfying:

$$\lambda_{\min}(\Sigma_t) \geq \frac{\sigma_{\min}^2(X)^2 \sigma_{\min}^2(Y)^2}{Bn^2},$$

where $\sigma_{\min}(X)$ and $\sigma_{\min}(Y)$ are the smallest singular values of the data matrix and target matrix respectively. (*Hint*: use the gradient formula from Theorem 1.4.1 and bound the covariance of the per-sample gradients from below using the singular value decomposition of X and Y.)

Problem 5.4 (C). Implement the negative curvature descent (Theorem 1.6.1) for the two-layer linear network of the chapter. Specifically:

(a) Initialise $W_1 = W_2 = 0$ (the saddle point).

(b) Compute the negative curvature direction v_- at the saddle using 20 steps of power iteration on the Hessian.

(c) Perform one negative curvature descent step with $t^* = \gamma/\rho$ (Theorem 1.6.1).

(d) Verify that the loss decreases by at least $\gamma^3/(6\rho^2)$.

(e) Compare to the number of SGD steps needed to achieve the same loss decrease.

Problem 5.5 (R). *Research problem*: The Åufinger–Ben Arous–Černý theorem (Theorem 1.3.1) is proved for isotropic Gaussian random fields. Design a numerical experiment to test whether the loss–index monotonicity of Corollary 1.3.1 holds for the empirical Hessian of a small transformer (2 layers, 4 heads, width 64) trained on a character-level language modelling task.

(a) Train the transformer to completion.

(b) Use the Lanczos algorithm to find the 50 largest and 50 smallest Hessian eigenvalues at various checkpoints during training.

(c) Compute the index (fraction of negative eigenvalues) at each checkpoint.

(d) Plot loss vs. index. Is the monotonicity approximately satisfied?

(e) What deviations from the isotropic prediction do you observe? Formulate a hypothesis for why they occur.

Chapter 2: Adaptive Optimisers

Problem 5.6 (C). Implement Adam and AdamW from scratch (no PyTorch optimiser classes) on the following problem:

- $L(w) = \frac{1}{2n}\|Xw - y\|^2 + \frac{\lambda}{2}\|w\|^2$, with $X \in \mathbb{R}^{100\times 200}$ random Gaussian, $y = Xw^* + \varepsilon$ for sparse $w^* \in \mathbb{R}^{200}$ (10 non-zero entries, $\varepsilon \sim \mathcal{N}(0, 0.01I)$), $\lambda = 0.01$.

For both Adam and AdamW (same hyperparameters: $\eta = 10^{-3}$, $\beta_1 = 0.9$, $\beta_2 = 0.999$):

(a) Run for 5000 steps. Plot training loss vs. steps.

(b) At convergence, compare $\|w_{\text{Adam}} - w^*\|$ and $\|w_{\text{AdamW}} - w^*\|$.

(c) Plot the effective weight decay $\eta\lambda w_i/(\hat{v}_i^{1/2} + \varepsilon)$ for Adam+L2 vs. $\eta\lambda w_i$ for AdamW, for each coordinate i. Verify that AdamW applies uniform decay while Adam+L2 applies coordinate-variable decay.

Problem 5.7 (A). Prove the following strengthening of Proposition 2.4.1 (non-equivalence of L2 and weight decay): for the Adam update, define the *effective regularisation coefficient* for parameter i as:

$$\lambda_i^{\text{eff}} = \frac{\eta\lambda}{\hat{v}_{t,i}^{1/2} + \varepsilon}.$$

Show that:

(a) For Adam+L2, λ_i^{eff} varies across coordinates by a factor up to $\max_i \hat{v}_{t,i}^{1/2} / \min_i \hat{v}_{t,i}^{1/2}$.

(b) For AdamW, $\lambda_i^{\text{eff}} = \eta\lambda$ (uniform) for all i.

(c) The ratio $\lambda_i^{\text{eff,L2}} / \lambda^{\text{eff,AdamW}}$ can be as small as $\varepsilon / (\max_i \hat{v}_{t,i}^{1/2})$ — essentially zero for large-gradient parameters.

Problem 5.8 (C). Reproduce the counter-example of Theorem 2.3.1 (Adam divergence) numerically:

(a) Implement the loss sequence $f_t(x) = Cx \cdot \mathbf{1}[t \equiv 0 \pmod 3] - x \cdot \mathbf{1}[t \not\equiv 0 \pmod 3]$ with $C = 3$, and run Adam ($\beta_1 = 0$, $\beta_2 = 0.99$, $\eta = 0.1$) for 300 steps.

(b) Plot w_t vs. t. Verify that $w_t \to \infty$.

(c) Run AMSGrad with the same parameters. Does it converge to $w^* = 0$?

(d) At what value of C does Adam transition from convergent to divergent? Find it numerically (try $C = 1.5, 2, 2.5, 3, 3.5$).

Problem 5.9 (A). Prove the following connection between the edge of stability and the condition number: for gradient descent on a quadratic $L(w) = \frac{1}{2} w^\top H w$ with $H = \operatorname{diag}(\lambda_1, \ldots, \lambda_d)$, $\lambda_1 \le \cdots \le \lambda_d$, and learning rate at the edge of stability $\eta = 2/\lambda_d$:

(a) Show that the sharpest component w_d oscillates with period 2 (neither converges nor diverges, but bounces).

(b) Compute the number of steps T for the flattest component w_1 to converge to $|w_{T,1}| \le \varepsilon |w_{0,1}|$. Express in terms of $\kappa = \lambda_d / \lambda_1$.

(c) Conclude that the edge-of-stability learning rate gives optimal convergence in the flat directions while keeping the sharp directions bounded.

(d) How does Adam's effective edge of stability (Corollary 2.6.1) improve on this?

Problem 5.10 (R). *Research problem*: The Schedule-Free Adam (Definition 2.7.1) uses a Cesàro average of iterates. The theoretical guarantee (Cesa-Bianchi et al., 2004) applies to the *online* setting. For the *offline* (fixed loss) non-convex setting:

(a) State precisely what convergence guarantee the online-to-batch conversion gives for Schedule-Free Adam in the non-convex case.

(b) Compare experimentally: train a ResNet-20 on CIFAR-10 with (i) Adam + cosine schedule, (ii) AdamW + cosine schedule, (iii) Schedule-Free Adam. Compare final test accuracy and training loss.

(c) Does Schedule-Free Adam find flatter minima (measured by $\lambda_{\max}(\nabla^2 L)$ at the final checkpoint) than Adam + cosine? If so, why?

Chapter 3: Sharpness-Aware Minimisation

Problem 5.11 (C). Implement PAC-Bayes bound computation for a small neural network:

(a) Train a 2-layer MLP (width 128, ReLU) on MNIST with SGD and with SAM.

(b) At convergence, compute the PAC-Bayes bound of Theorem 3.2.1 for both models, using $Q = \mathcal{N}(w^*, \rho^2 I/d)$ with $\rho = 0.01$ and $P = \mathcal{N}(0, I)$.

(c) Compute the three terms of the bound separately: training loss, $\mathbb{E}_{\varepsilon\sim Q}[L(w^*+\varepsilon)]-L(w^*)$ (sharpness), and $\mathrm{KL}(Q\|P)/(n)$.

(d) Compare with the actual test error. Which algorithm has a tighter bound?

Problem 5.12 (A). Prove the following strengthening of Proposition 3.4.1 (approximation error of SAM): for the k-th order Taylor approximation of the inner maximiser, the gap between the k-th order perturbation $\hat{\varepsilon}^{(k)}$ and the exact maximiser ε^* satisfies:

$$L(w+\varepsilon^*) - L(w+\hat{\varepsilon}^{(k)}) \leq \frac{\ell\rho^{k+1}}{(k+1)!},$$

where ℓ is the k-th order Lipschitz constant of L. (*Hint*: use the Taylor series with Lagrange remainder and the fact that $\|\varepsilon\| \leq \rho$.)

Problem 5.13 (C). Implement GSAM (Definition 3.6.2) and compare to SAM on the following problem: $L(w) = \frac{1}{4}\|Xw-y\|^4 + 10^{-2}(w_1^2 + 100w_2^2)$ (non-convex, sharp minimum).

(a) Plot the loss landscape.

(b) Run GD, SAM ($\rho = 0.1$), and GSAM ($\rho = 0.1$, $\gamma = 0.1$) for 500 steps.

(c) At convergence, compute: training loss, sharpness $\lambda_{\max}(H)$, and the PAC-Bayes generalisation bound.

(d) Which algorithm finds the flattest minimum? Does flatness correlate with the generalisation bound?

Problem 5.14 (A). Prove Proposition 3.7.1 (SAM and SWA target the same region) rigorously in the following special case:

(a) Let $L(w) = \frac{1}{2}w^\top Hw$ (quadratic). Show that the SWA iterate $\bar{w}_T = \frac{1}{T-T_0}\sum_{t=T_0}^{T} w_t$ with a cyclic learning rate satisfying $\eta_t = \eta_{\max}\cos^2(\pi t/(2T_{\text{cycle}}))$ converges to the posterior mean $\mathbb{E}_{\mathcal{N}(w^*,\rho^2H^{-1})}[w] = w^*$.

(b) Show that SAM with perturbation radius ρ gives an effective update that minimises $\max_{\|\varepsilon\|\leq\rho} L(w+\varepsilon) = L(w) + \rho\|\nabla L(w)\|$, and that this is equivalent to minimising the posterior expected loss under $Q = \mathcal{N}(w, \rho^2H^{-1})$ to first order in ρ.

(c) Conclude: both methods are solving the same PAC-Bayes objective, one via averaging and one via worst-case perturbation.

Problem 5.15 (R). *Research problem*: The SAM generalisation bound (Theorem 3.5.1) uses a Gaussian posterior centred at w^*_{SAM}. A more refined bound might use a posterior centred at the *mode* of the Gibbs posterior $p(w|S) \propto e^{-nL_{\text{train}}(w)}$.

(a) Show that the Gibbs posterior mode satisfies $w^*_{\text{Gibbs}} = w^*_{\text{SAM}}$ when the perturbation ball coincides with a level set of $p(w|S)$.

(b) For a logistic regression model with $n = 1000$ samples, compute the PAC-Bayes bound for three posteriors: $\mathcal{N}(w^*, 0.01I)$, $\mathcal{N}(w^*, 0.1I)$, $\mathcal{N}(w^*, I)$. Which gives the tightest bound?

(c) What does the optimal posterior variance σ^2 depend on, and how would you estimate it in practice without evaluating the full Fisher matrix?

Chapter 4: Plasticity and Continual Learning

Problem 5.16 (**C**). Implement the three-task continual learning example from Section 4.5.3:

(a) Implement fine-tuning, EWC ($\lambda = 1$), and GEM on the three-task quadratic problem of Example 4.7.2, with $w \in \mathbb{R}^3$ and tasks $L_k(w) = \frac{1}{2}\|w - e_k\|^2$.

(b) For each algorithm, plot the trajectory $\{w^{(k)}\}_{k=1}^3$ in $\mathbb{R}^3$.

(c) Compute the final losses $L_1(w^{(3)}), L_2(w^{(3)}), L_3(w^{(3)})$ and the plasticity functional $\mathcal{P}(w^{(3)})$ (assuming full-rank weights, so $\mathcal{P} = 1 - \phi_{\text{dead}}$).

(d) Plot the Pareto curve (stability vs. plasticity) for EWC as λ varies from 0 to ∞. Verify it matches Table 4.1.

Problem 5.17 (**A**). Prove Proposition 4.6.1 (continual learning as Wasserstein flow) in detail for the special case of two tasks with Gaussian posteriors.

(a) Let $L_1(w) = \frac{1}{2}\|w - a\|^2$, $L_2(w) = \frac{1}{2}\|w - b\|^2$ with $a \neq b \in \mathbb{R}^d$.

(b) Show that the Gibbs posterior after task 1 is $\pi_1 = \mathcal{N}(a, TI)$ for some temperature T.

(c) Show that the Wasserstein gradient flow of $\mathcal{F}_2(\mu) = \int L_2\, d\mu + \beta\,\mathrm{KL}(\mu\|\pi_1)$ is the Ornstein–Uhlenbeck process: $\dot{w} = -(w - b) - \beta(w - a) = -((1 + \beta)w - b - \beta a)$.

(d) Solve the ODE explicitly. What is the fixed point? How does β control the trade-off between the two tasks?

(e) Verify that for $\beta \to \infty$, the fixed point approaches a (complete forgetting prevention), and for $\beta \to 0$, it approaches b (complete forgetting).

Problem 5.18 (**C**). Implement the dormancy spiral simulation of Section 4.9 (toy model):

(a) Build a 2-layer ReLU network (width 50) trained with Adam on the toy problem: $X \in \mathbb{R}^{20\times 1000}$, $y = \mathrm{ReLU}(W^* X)$ for diagonal W^* with entries $1, 0.1, 0.1, \ldots, 0.1$ (one strong feature, 19 weak features).

(b) Train for 5000 steps. At each 100 steps, compute: dead fraction ϕ_{dead}, effective rank $\mathrm{rank}_{\text{eff}}(W)$, and minimum second moment $\min_i \hat{v}_{t,i}$.

(c) Plot all three quantities over training. Do you observe the dormancy spiral (rank collapse $\to$ dead neurons $\to$ gradient concentration)?

(d) Apply ReDo (reset dead neurons every 500 steps) and repeat. How does this change the trajectories?

Problem 5.19 (**A**). Prove the following quantitative bound on the rate of plasticity loss: under the assumption that the gradient variance in dead-neuron directions satisfies $\mathrm{Var}[\nabla_{W_i} L] \leq \sigma^2_{\text{dead}}$ (small, since dead neurons contribute zero gradient), show that for Adam with hyperparameters $(\eta, \beta_1, \beta_2, \varepsilon)$:

$$\mathbb{P}\Big[\phi^{(l)}_{\text{dead}}(w_T) \geq \phi^{(l)}_{\text{dead}}(w_0) + \Delta\Big] \leq \exp\left(-\frac{\Delta^2 d_l}{2(\sigma^2_{\text{dead}} T\eta^2/\varepsilon^2 + \Delta)}\right).$$

(*Hint*: model the change in each neuron's activation as a random walk with step size bounded by the Adam update magnitude, and apply Azuma's inequality.)

Problem 5.20 (**R**). *Research problem*: Design an algorithm that achieves high sharpness-adjusted plasticity $\Pi(w^*) = \mathcal{P}(w^*)/(1 + \alpha\lambda_{\max}(\nabla^2 L(w^*)))$ simultaneously.

(a) Show that SAM alone (without plasticity control) achieves small $\lambda_{\max}$ but may have small $\mathcal{P}$ (due to Adam-induced rank collapse in AdamSAM).

(b) Show that ReDo alone (without sharpness control) achieves large $\mathcal{P}$ but may have large $\lambda_{\max}$ (no flatness seeking).

(c) Propose a combined algorithm (SAM + ReDo, or a new algorithm) that targets both. Specify: (i) how often to apply each component, (ii) how to set the hyperparameters (ρ, λ, τ), (iii) what theoretical guarantee you would need to prove for the combined algorithm.

(d) Test your proposed algorithm on a 5-task continual learning benchmark (e.g., Split CIFAR-10). Measure both sharpness and plasticity at each task boundary.

Cross-Chapter Problems

Problem 5.21 (**A**). *Hessian through all four chapters.* For the two-layer linear network $L(W_1, W_2) = \frac{1}{2n}\|W_2W_1X - Y\|_F^2$ with the specific values of Section 1.8 ($d_0 = d_2 = k = 2$, $n = 4$, X and Y as given):

(a) **Chapter 1**: Compute the Hessian at the saddle $(W_1, W_2) = (0, 0)$ and verify its index is 4.

(b) **Chapter 2**: Compute Adam's edge of stability threshold at the global minimum W^*.

(c) **Chapter 3**: Compute the SAM perturbation direction $\hat{\varepsilon}$ at the point $(W_1, W_2) = (0.5W_1^*, 0.5W_2^*)$ (halfway to the minimum).

(d) **Chapter 4**: Compute the EWC importance weight F_{ii} for the diagonal Fisher at the global minimum W^*.

Problem 5.22 (**C**). *Algorithm comparison on a standard benchmark.* Train a ResNet-18 on CIFAR-100 using each of the following algorithms: (i) SGD + momentum, (ii) Adam, (iii) AdamW, (iv) SAM + SGD, (v) SAM + Adam. For each, record at convergence:

(a) Training loss, test accuracy (standard metrics).

(b) Sharpness $\lambda_{\max}(\nabla^2 L_{\text{train}})$ (via 20 power iterations).

(c) Effective rank of each layer's weight matrix.

(d) PAC-Bayes bound (using $\rho = 0.01$).

Organise results in a table and discuss: is there a consistent relationship between sharpness, effective rank, and generalisation across algorithms?

Problem 5.23 (**R**). *Unified theory of optimiser choice.* Based on the four chapters, propose a decision tree for choosing an optimiser:

(a) For each combination of (stationary/non-stationary task setting) × (generalisation/speed primary goal) × (small/large model), which algorithm from the volume do you recommend?

(b) Justify each recommendation using theorems from the relevant chapter.

(c) Identify the one combination for which no good algorithm exists yet, and formulate it as a precise open problem.

Closing Remarks: What We Know and What We Don't

Mathematics is the art of giving the same name to different things.
— Henri Poincaré

The four chapters of this volume have developed a mathematical theory of optimisation for deep learning, and Chapter 5 has synthesised the connections. What remains is to be honest about the limits of what has been achieved, and about the gap between the theory developed here and the practice of training large neural networks.

What the Theory Gets Right

The theory developed in this volume makes several predictions that are borne out by experiment:

1. The loss landscape at convergence is dominated by minima, not saddle points. Theorem 1.3.1 (Åufinger–Ben Arous–Černý) proves this for isotropic Gaussian fields, and the empirical evidence for trained networks (Goodfellow et al. 2015, Dauphin et al. 2014) is consistent. The practical consequence: gradient descent converges in practice because the loss landscape is geometrically benign at the bottom — not because the algorithm is clever at escaping saddle points.

2. Adam converges differently from SGD. Theorems 2.5.1 and 2.7.1 prove that Adam's implicit bias is toward ℓ^∞-sparse solutions (linear models) and low-effective-rank solutions (matrix problems), while SGD's is toward ℓ_2-dense, higher-rank solutions. The empirical evidence (Table 4.1) confirms this: Adam-trained networks have systematically lower effective rank and higher dead neuron fraction than SGD-trained ones. The implication — that Adam's implicit bias trades long-horizon plasticity for short-horizon convergence speed — is a novel prediction of the theory that has not been fully tested at LLM scale.

3. Flat minima generalise better, and SAM finds them. Theorem 3.5.1 gives a rigorous PAC-Bayes justification for the sharpness–generalisation connection. The empirical evidence (Keskar et al. 2017, Foret et al. 2021) is strong. The theoretical gap: the PAC-Bayes bound is not tight (as illustrated in Section 5.4.2), so the theory does not predict the magnitude of the generalisation improvement from SAM, only its direction.

4. EWC is Bayesian sequential inference, and GEM projects gradients correctly. The derivations in Chapter 4 are mathematically rigorous. The practical predictions — that diagonal Fisher EWC is a good approximation for small task shifts, and that GEM's gradient projection is necessary but not sufficient for preventing forgetting — are consistent with the continual learning benchmarks.

What the Theory Gets Wrong

1. The isotropic Gaussian field model is not neural networks. Theorem 1.3.1 is proved for isotropic Gaussian fields. Real neural network losses are highly anisotropic, non-Gaussian, and have specific structure from the architecture (layer normalisation, residual connections, attention). The qualitative predictions (high-index saddles at high loss, minima at low loss) appear to be correct, but the quantitative predictions (exact complexity function $\Theta_k(u)$) are not. Conjecture B (anisotropic loss–index correlation) remains unproved.

2. The Adam convergence rate of $O(T^{-1/4})$ is too pessimistic. Theorem 2.9.1 gives a $T^{-1/4}$ rate for Adam, while SGD achieves $T^{-1/2}$. In practice, Adam is consistently faster than SGD in wall-clock time. The $T^{-1/4}$ bound is a worst-case over adversarial gradient sequences and is not tight for the smooth, structured losses encountered in practice. This is the most significant gap between theory and practice in the volume: the algorithm that is used everywhere has a weaker theoretical guarantee than the algorithm that nobody uses.

3. The PAC-Bayes bound is vacuous for large models. As illustrated in Section 5.4.2, the PAC-Bayes bound for a typical transformer is vacuous (gives $L_{\text{pop}} \leq 6$ for a $[0,1]$-valued loss). The $\mathrm{KL}(Q\|P)/n$ term is enormous because the model has $d \sim 10^{10}$ parameters, making the KL divergence proportional to $d\log(d\sigma^2/\rho^2) \sim 10^{10}$, far larger than n (even for $n = 10^{12}$). The PAC-Bayes framework is theoretically motivated but practically vacuous for modern foundation models. New ideas — perhaps based on the intrinsic dimensionality of the learned representation, or on distribution-specific rather than worst-case bounds — are needed.

4. The dormancy spiral is empirically consistent but unproved. Conjecture 4.9.1 describes a mechanism for plasticity loss that is consistent with all available evidence. But it is a conjecture, not a theorem, and the absence of a proof means the mechanism could be wrong (or right for the wrong reasons). The toy model of Section 4.9 shows that the mechanism is at least plausible; formalising it is the most important open problem in Chapter 4.

The Path Forward: Part IV

This volume is the third in the Mathematics of Deep Learning series. Part IV (forthcoming) will address the subjects identified as open in this volume:

Chapter 1 of Part IV (Statistical Physics of the Loss Landscape) will develop the rigorous RMT analysis of the Hessian at trained minima, including the free energy calculations (Section A.3), the replica theory of spin glasses as applied to deep networks, and the Gardner transition in the overparameterised regime.

Chapter 2 of Part IV (Information Geometry and Natural Gradient) will develop the complete information-geometric theory of adaptive optimisers, including K-FAC, Shampoo, and Muon as approximations to the natural gradient on different Riemannian manifolds.

Chapter 3 of Part IV (Geometry of Generalisation) will address the gap between PAC-Bayes bounds and practised performance for large models, developing bounds based on intrinsic dimensionality and the geometry of the interpolating manifold.

Chapter 4 of Part IV (Dynamical Theory of Continual Learning) will prove (or disprove) the dormancy spiral conjecture, develop the full Wasserstein gradient flow theory for finite particle systems, and connect the mathematical framework to the neuroscientific complementary learning systems theory.

The mathematics of deep learning is a young field. The results in this volume represent the current frontier: rigorous where possible, conjectural where necessary, and honest about the difference. The open problems identified here are not failures of the theory but invitations — to the reader, to the student, to the researcher — to push the frontier further.

Silvano Salvador
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Bibliographic Notes

Chapter 1

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Appendix A: Random Matrix Theory Essentials

This appendix provides a self-contained review of the random matrix theory results used throughout the volume. It is not a substitute for the comprehensive treatment in the Statistical Physics companion volume, but it makes the present volume self-contained for readers who arrive from Chapter 1 without prior exposure to RMT.

A.1 Matrix Ensembles

Definition 5.37 (Gaussian Orthogonal Ensemble)**.** A symmetric random matrix $M \in \mathbb{R}^{d\times d}$ belongs to the *Gaussian Orthogonal Ensemble* (GOE) if:

$$M_{ij} = M_{ji} \sim \mathcal{N}(0, 1/d) \quad i < j, \qquad M_{ii} \sim \mathcal{N}(0, 2/d).$$

The factor $1/d$ ensures that the bulk of the spectrum remains $O(1)$ as $d \to \infty$. The GOE is invariant under orthogonal conjugation: if O is a random orthogonal matrix independent of M, then $OMO^\top \overset{d}{=} M$.

Definition 5.38 (Wishart / Marchenko–Pastur matrix)**.** Let $X \in \mathbb{R}^{n\times d}$ have i.i.d. entries $X_{ij} \sim \mathcal{N}(0, 1/n)$. The *sample covariance matrix* $W = X^\top X \in \mathbb{R}^{d\times d}$ follows the *Wishart distribution* $\mathcal{W}_d(n, I/n)$. As $d, n \to \infty$ with $\gamma = d/n \to c > 0$, the empirical spectral distribution converges to the *Marchenko–Pastur law* with parameter γ:

$$\rho_{\mathrm{MP}}(\lambda; \gamma) = \frac{\sqrt{(\lambda_+ - \lambda)(\lambda - \lambda_-)}}{2\pi\gamma\lambda} \cdot \mathbf{1}_{[\lambda_-, \lambda_+]}(\lambda),$$

where $\lambda_\pm = (1 \pm \sqrt{\gamma})^2$ are the upper and lower edges of the support. When $\gamma > 1$ (more features than samples), there is an additional point mass of weight $1 - 1/\gamma$ at zero.

Remark 5.39 (Connection to neural network Hessians). The Hessian of a trained neural network with d parameters trained on n samples has an empirical spectral distribution approximately given by:

$$\rho_H \approx (1 - \varepsilon)\, \rho_{\mathrm{MP}}(\cdot; n/d) + \varepsilon\, \rho_{\mathrm{out}},$$

where ρ_{out} is a discrete measure on $r \ll d$ outlier eigenvalues. The bulk follows Marchenko–Pastur with aspect ratio n/d (samples-to-parameters ratio); the outliers correspond to the "sharpest" directions of the loss, associated with the most important features. This structure is documented empirically by Papyan (2018) and Ghorbani, Krishnan, and Xiao (2019).

A.2 Key Results

Theorem 5.40 (Wigner semicircle law)**.** *Let $M^{(d)}$ be a $d \times d$ GOE matrix. The empirical spectral distribution $\mu_d = \frac{1}{d}\sum_i \delta_{\lambda_i(M^{(d)})}$ converges almost surely to:*

$$\rho_{\mathrm{sc}}(\lambda) = \frac{1}{2\pi}\sqrt{4 - \lambda^2}\, \mathbf{1}_{|\lambda|\le 2}.$$

Theorem 5.41 (Baik–Ben Arous–Péché (BBP) phase transition)**.** *Let M be a $d\times d$ GOE matrix and let $A = M+\mathrm{diag}(\theta_1,\dots,\theta_r,0,\dots,0)$ be a rank-r perturbation. The outlier eigenvalues of A satisfy:*

$$\lambda_i(A) \to \begin{cases} \theta_i + 1/\theta_i & \text{if } \theta_i > 1 \\ 2 & \text{if } \theta_i \le 1 \end{cases} \quad \text{almost surely as } d\to\infty.$$

When $\theta_i > 1$, the i-th eigenvalue pops out *of the bulk; when $\theta_i \le 1$, it remains inside the bulk and is not separately identifiable.*

Remark 5.42 (Implication for Hessian outliers). The BBP transition explains the observed outlier structure of neural network Hessians: the "important" directions of the loss (corresponding to directions of strong curvature in parameter space) produce outlier eigenvalues that pop out of the Marchenko–Pastur bulk. The threshold $\theta_i = 1$ corresponds to a signal-to-noise ratio of 1 in the gradient covariance structure. Below this threshold, the direction is indistinguishable from noise; above it, it produces an identifiable outlier.

A.3 Free Probability and Operator Addition

When two large random matrices A and B are "freely independent" (a notion analogous to statistical independence for matrices), their empirical spectral distributions combine via *free convolution* $\boxplus$:

$$\mu_{A+B} = \mu_A \boxplus \mu_B.$$

This allows computation of the spectral distribution of $\nabla^2 L = \nabla^2 L_{\text{bulk}} + \nabla^2 L_{\text{outlier}}$ when the two components are approximately free. In practice, the Hessian of a deep network is approximately the sum of a Wishart-type matrix (from the sample Gram matrix of gradients) and a low-rank correction (from the curvature in the output layer), and their free convolution gives the observed bulk-plus-outliers spectrum.

A.4 Largest Eigenvalue Distributions

The largest eigenvalue of a GOE matrix concentrates around 2 (the upper edge of the semicircle) with fluctuations of order $d^{-2/3}$ governed by the Tracy–Widom distribution F_1:

$$\mathbb{P}\Big[d^{2/3}(\lambda_{\max}(M) - 2) \le s\Big] \to F_1(s).$$

For the Marchenko–Pastur ensemble (Wishart matrix), the largest eigenvalue concentrates around $\lambda_+ = (1+\sqrt{\gamma})^2$ with the same $d^{-2/3}$ fluctuations and Tracy–Widom law (F_2 in the complex case).

Remark 5.43 (Implication for the edge of stability). The edge-of-stability phenomenon (Section 2.6) involves the sharpness $\ell_t = \lambda_{\max}(\nabla^2 L(w_t))$. The Tracy–Widom concentration around λ_+ means that the sharpness is *deterministically* close to its bulk upper edge for large d, with fluctuations of order $d^{-2/3}$. The outlier eigenvalues (from the BBP transition) contribute additional sharpness above the bulk edge. The edge-of-stability attractor at $\ell^* \approx 2/\eta$ (for SGD) thus has two components: the bulk contribution $\lambda_+ = (1+\sqrt{\gamma})^2$ and the outlier contribution, which must both satisfy the stability condition.

A.5 Numerical Exercises on RMT

Exercise 5.11. Generate a 500×500 GOE matrix in any numerical language (Python/MATLAB).

(a) Plot the histogram of eigenvalues. Overlay the semicircle density ρ_{sc}.

(b) Compute $\lambda_{\max}$ and $\lambda_{\min}$. Are they close to ± 2?

(c) Add a rank-1 perturbation $\theta e_1 e_1^\top$ with $\theta = 1.5$. Does the largest eigenvalue pop out of the bulk? Compare with the BBP prediction $\theta + 1/\theta$.

(d) Repeat with $\theta = 0.5$. Does the eigenvalue pop out?

Exercise 5.12. Generate a Wishart matrix $W = X^\top X$ with $X \in \mathbb{R}^{200 \times 500}$ (aspect ratio $\gamma = 500/200 = 2.5$).

(a) What are the theoretical bounds $\lambda_\pm$? Verify numerically.

(b) Plot the empirical spectral distribution and overlay the Marchenko–Pastur density.

(c) Add a rank-3 perturbation with strengths $\theta_1 = 2, \theta_2 = 0.8, \theta_3 = 0.3$. Which, if any, pop out of the bulk?

Exercise 5.13 (Connection to neural network Hessians)**.** Train a small two-layer ReLU network (width 64, depth 2) on a subset of MNIST (1000 samples). After training, compute the Hessian spectrum using the Lanczos algorithm (available in PyTorch via `torch.lobpcg` or the `pyhessian` library).

(a) Plot the empirical spectral density. Does it show a bulk-plus-outliers structure?

(b) Estimate the aspect ratio $\gamma = n/d$ and compare the bulk edge with the Marchenko–Pastur prediction $(1 + \sqrt{\gamma})^2$.

(c) How many outlier eigenvalues are there? How does this compare to the output dimension of the network?

Appendix B: Notation and Conventions

B.1 Sets and Spaces

Symbol	Meaning
$\mathbb{R}^d$	d-dimensional Euclidean space
$\mathcal{B}(w, r)$	closed ℓ_2 ball of radius r centred at w
S^{d-1}	unit sphere in $\mathbb{R}^d$
$S^{d-1}(\sqrt{d})$	sphere of radius $\sqrt{d}$ in $\mathbb{R}^d$
$\mathcal{W}_2(\mathbb{R}^d)$	Wasserstein-2 space of probability measures on $\mathbb{R}^d$
$\mathcal{N}(\mu, \Sigma)$	Gaussian distribution with mean μ, covariance Σ
Uniform(S)	uniform distribution on set S
$[d]$	the set $\{1, 2, \ldots, d\}$

B.2 Matrix Operations

Symbol	Meaning
$\|A\|_F$	Frobenius norm: $\sqrt{\sum_{ij} A_{ij}^2}$
$\|A\|$ or $\|A\|_2$	spectral norm (largest singular value)
$\|A\|_*$	nuclear norm (sum of singular values)
$\mathrm{tr}(A)$	trace: $\sum_i A_{ii}$
$\mathrm{rank}(A)$	rank (number of nonzero singular values)
$\mathrm{rank}_{\mathrm{eff}}(A)$	effective rank (Definition 4.2.2)
$\lambda_i(A)$	i-th eigenvalue of symmetric A (ascending order unless noted)
$\lambda_{\min}(A)$, $\lambda_{\max}(A)$	smallest and largest eigenvalues
$\sigma_i(A)$	i-th singular value of A (descending order)
$A \succ 0$, $A \succeq 0$	positive definite, positive semi-definite
$\mathrm{diag}(v)$	diagonal matrix with vector v on diagonal
$v_1 \odot v_2$	element-wise (Hadamard) product
$A \otimes B$	Kronecker product
Π_S	orthogonal projection onto subspace S

B.3 Calculus and Optimisation

Symbol	Meaning
$\nabla f(w)$	gradient of f at w: vector in $\mathbb{R}^d$
$\nabla^2 f(w) = \nabla^2 f(w)$	Hessian of f at w: matrix in $\mathbb{R}^{d\times d}$
$\nabla^2 f(w)[v, v]$	second directional derivative: $v^\top \nabla^2 f(w) v$
$D_\psi(w, w')$	Bregman divergence generated by ψ
$\mathrm{prox}_{\eta f}(w)$	proximal operator: $\arg\min_u \{f(u) + \|u - w\|^2/(2\eta)\}$
$\partial f(w)$	subdifferential of convex f at w
ℓ-smooth	f satisfies $\|\nabla f(w) - \nabla f(w')\| \le \ell \|w - w'\|$
ρ-Hessian-Lipschitz	$\|\nabla^2 f(w) - \nabla^2 f(w')\| \le \rho \|w - w'\|$
Δ_f	initial suboptimality $f(w_0) - f^*$
w^*	a critical point or minimiser of f (context-dependent)

B.4 Probability and Statistics

Symbol	Meaning
$\mathbb{E}[X]$	expectation of random variable X
$\mathbb{E}_{w\sim Q}[f(w)]$	expectation of $f(w)$ when $w \sim Q$
$\mathbb{P}[E]$	probability of event E
$\mathrm{Var}[X]$	variance of X
$\mathrm{Cov}[X, Y]$	covariance of X and Y
$\mathrm{KL}(Q\|P)$	KL divergence from P to Q: $\int \log(dQ/dP)\, dQ$
$W_2(\mu, \nu)$	Wasserstein-2 distance between measures μ, ν
$\xrightarrow{d}$	convergence in distribution
$\xrightarrow{a.s.}$	almost sure convergence
$X \overset{d}{=} Y$	equal in distribution

B.5 Deep Learning Notation

Symbol	Meaning
$w \in \mathbb{R}^d$	model parameters (flattened)
$W^{(l)} \in \mathbb{R}^{d_l \times d_{l-1}}$	weight matrix of layer l
$f_w : \mathbb{R}^{d_0} \to \mathbb{R}^{d_L}$	network function
$L(w)$ or $L_{\text{train}}(w)$	training loss
$L_{\text{pop}}(w)$	population (test) loss
$\ell(f_w(x), y)$	per-sample loss
n	number of training samples
B	mini-batch size
η	learning rate
T	number of training steps
$g_t = \nabla L(w_t)$	gradient at step t
$\hat{g}_t$	mini-batch gradient estimate
m_t, v_t	first and second moment estimates (Adam)
$\hat{m}_t, \hat{v}_t$	bias-corrected moment estimates (Adam)
β_1, β_2	Adam momentum coefficients
ε	Adam numerical stabiliser ($\approx 10^{-8}$)
λ	weight decay coefficient or regularisation strength
ρ	SAM perturbation radius
$\phi_{\text{dead}}^{(l)}$	dead neuron fraction at layer l
$\mathcal{P}(w)$	plasticity functional
$F(w)$	Fisher information matrix
$H = \nabla^2 L(w)$	Hessian of loss
$\ell^* = \lambda_{\max}(H)$	sharpness at w

B.6 Standard Identities

The following identities are used repeatedly without proof.

Fisher identity: For a model $p_w(y|x)$:

$$\mathbb{E}_{y|x}[\nabla_w \log p_w(y|x)] = 0, \qquad F(w) = \mathbb{E}\Big[(\nabla_w \log p_w)(\nabla_w \log p_w)^\top\Big] = -\mathbb{E}\big[\nabla_w^2 \log p_w\big]\,.$$

Quadratic form: For $A \succ 0$ and $\varepsilon \sim \mathcal{N}(0, \sigma^2 I)$:

$$\mathbb{E}[\varepsilon^\top A \varepsilon] = \sigma^2 \operatorname{tr}(A).$$

KL divergence for Gaussians: For $P = \mathcal{N}(\mu_P, \Sigma_P)$ and $Q = \mathcal{N}(\mu_Q, \Sigma_Q)$:

$$\mathrm{KL}(Q\|P) = \frac{1}{2}\left[\operatorname{tr}(\Sigma_P^{-1}\Sigma_Q) + (\mu_P - \mu_Q)^\top \Sigma_P^{-1}(\mu_P - \mu_Q) - d + \log\frac{\det \Sigma_P}{\det \Sigma_Q}\right].$$

Stein's lemma: For $\varepsilon \sim \mathcal{N}(0, \Sigma)$ and smooth f:

$$\mathbb{E}[\varepsilon f(\varepsilon)] = \Sigma\, \mathbb{E}[\nabla f(\varepsilon)].$$

Appendix C: Algorithms Reference

This appendix collects complete pseudocode for all algorithms discussed in the volume, with implementation notes. All algorithms are presented in a unified notation.

C.1 Gradient Descent and Variants

Algorithm 4 Vanilla Gradient Descent (GD)

Require: L, η, w_0, T

for $t = 1$ to T **do**
  $g_t \leftarrow \nabla L(w_{t-1})$ ▷ Full gradient
  $w_t \leftarrow w_{t-1} - \eta g_t$
end for
return w_T

Algorithm 5 Stochastic Gradient Descent (SGD)

Require: L, η, w_0, T, batch size B

for $t = 1$ to T **do**
  Sample mini-batch $\mathcal{B}_t \subset [n]$ with $|\mathcal{B}_t| = B$
  $g_t \leftarrow \frac{1}{B} \sum_{i \in \mathcal{B}_t} \nabla L_i(w_{t-1})$
  $w_t \leftarrow w_{t-1} - \eta_t g_t$
end for
return w_T (or $\bar{w}_T = \frac{1}{T} \sum_{t=1}^{T} w_t$ for convex losses)

Implementation note: the learning rate η_t is typically constant for first phase, then decayed (cosine, polynomial). Gradient clipping ($g_t \leftarrow g_t \cdot \min(1, c/\|g_t\|)$ for clip norm c) is standard in LLM training.

Algorithm 6 Perturbed Gradient Descent (PGD) — Theorem 1.5.1

Require: L, η, r, $g_{\min}$, perturbation frequency $\mathcal{T}$, w_0, T

for $t = 1$ to T **do**
  $g_t \leftarrow \nabla L(w_{t-1})$
  if $\|g_t\| \le g_{\min}$ **and** $t \in \mathcal{T}$ **then**
    $\xi_t \sim \text{Uniform}(\mathcal{B}(0, r))$
  else
    $\xi_t \leftarrow 0$
  end if
  $w_t \leftarrow w_{t-1} - \eta g_t + \xi_t$
end for
return w_T

Recommended parameters (from Theorem 1.5.1): $\eta = 1/(10\ell)$, $r = \delta\gamma^2/(10\rho\ell d)$, $g_{\min} = (\delta\gamma^2/(10\rho))^{1/2}$, $\mathcal{T} = \{t : t \equiv 0 \pmod{\lceil 1/\eta\gamma \rceil}\}$.

C.2 Adaptive Optimisers

Algorithm 7 Adam — Definition 2.2.2

Require: L, η, β_1, β_2, ε, w_0, T

$m_0 \leftarrow 0$, $v_0 \leftarrow 0$
for $t = 1$ to T **do**
  $g_t \leftarrow \nabla L(w_{t-1})$ (or stochastic estimate)
  $m_t \leftarrow \beta_1 m_{t-1} + (1-\beta_1) g_t$
  $v_t \leftarrow \beta_2 v_{t-1} + (1-\beta_2) g_t^2$ ▷ Element-wise square
  $\hat{m}_t \leftarrow m_t / (1-\beta_1^t)$
  $\hat{v}_t \leftarrow v_t / (1-\beta_2^t)$
  $w_t \leftarrow w_{t-1} - \eta \hat{m}_t / (\sqrt{\hat{v}_t} + \varepsilon)$
end for
return w_T

Standard hyperparameters: $\beta_1 = 0.9$, $\beta_2 = 0.999$, $\varepsilon = 10^{-8}$, $\eta = 10^{-3}$ to 10^{-4} (problem-dependent). For LLM training: $\eta = 10^{-4}$ with cosine schedule, $\beta_2 = 0.95$ (faster forgetting of old second moments), $\varepsilon = 10^{-6}$.

Algorithm 8 AMSGrad — Definition 2.3.1

Require: L, η, β_1, β_2, ε, w_0, T

$m_0 \leftarrow 0$, $v_0 \leftarrow 0$, $\hat{v}_0 \leftarrow 0$
for $t = 1$ to T **do**
  $g_t \leftarrow \nabla L(w_{t-1})$
  $m_t \leftarrow \beta_1 m_{t-1} + (1-\beta_1) g_t$
  $v_t \leftarrow \beta_2 v_{t-1} + (1-\beta_2) g_t^2$
  $\hat{v}_t \leftarrow \max(\hat{v}_{t-1}, v_t)$ ▷ Coordinate-wise maximum
  $w_t \leftarrow w_{t-1} - \eta m_t / (\sqrt{\hat{v}_t} + \varepsilon)$
end for
return w_T

Algorithm 9 AdamW — Definition 2.4.1

Require: L, η, β_1, β_2, ε, λ, w_0, T

$m_0 \leftarrow 0$, $v_0 \leftarrow 0$
for $t = 1$ to T **do**
  $g_t \leftarrow \nabla L(w_{t-1})$ ▷ Gradient of task loss only, no weight decay
  $m_t \leftarrow \beta_1 m_{t-1} + (1-\beta_1) g_t$
  $v_t \leftarrow \beta_2 v_{t-1} + (1-\beta_2) g_t^2$
  $\hat{m}_t \leftarrow m_t / (1-\beta_1^t)$, $\hat{v}_t \leftarrow v_t / (1-\beta_2^t)$
  $w_t \leftarrow (1 - \eta\lambda) w_{t-1} - \eta \hat{m}_t / (\sqrt{\hat{v}_t} + \varepsilon)$ ▷ Weight decay applied separately
end for
return w_T

Key difference from Adam+L2: the weight decay $-\eta\lambda w$ is applied *before* the gradient update, not included in g_t. This prevents the weight decay from being scaled by the preconditioner.

Algorithm 10 Schedule-Free Adam — Definition 2.7.1

Require: L, η, β_1, β_2, ε, w_0, T

$z_0 \leftarrow w_0$, $x_0 \leftarrow w_0$
$m_0 \leftarrow 0$, $v_0 \leftarrow 0$
for $t = 1$ to T **do**
  $g_t \leftarrow \nabla L(x_{t-1})$ ▷ Gradient at checkpoint, not at z
  $m_t \leftarrow \beta_1 m_{t-1} + (1-\beta_1) g_t$
  $v_t \leftarrow \beta_2 v_{t-1} + (1-\beta_2) g_t^2$
  $P_t \leftarrow \operatorname{diag}(\sqrt{\hat{v}_t} + \varepsilon)$
  $z_t \leftarrow z_{t-1} - \eta P_t^{-1} g_t$ ▷ Aggressive iterate
  $x_t \leftarrow \left(1 - \frac{1}{t}\right) x_{t-1} + \frac{1}{t} z_t$ ▷ Averaged checkpoint
end for
return x_T ▷ Return averaged checkpoint, not last iterate

C.3 Sharpness-Aware Minimisation

Algorithm 11 SAM — Algorithm 3.1

Require: L, η, ρ, w_0, T

for $t = 1$ to T **do**
  Sample mini-batch $\mathcal{B}_t$
  $g_t \leftarrow \nabla_w L_{\mathcal{B}_t}(w_{t-1})$ ▷ First gradient for perturbation
  $\hat{\varepsilon}_t \leftarrow \rho \cdot g_t / \|g_t\|$ ▷ Perturbation direction
  $\tilde{g}_t \leftarrow \nabla_w L_{\mathcal{B}_t}(w_{t-1} + \hat{\varepsilon}_t)$ ▷ Second gradient for update
  $w_t \leftarrow w_{t-1} - \eta \tilde{g}_t$
end for
return w_T

Algorithm 12 ASAM (Adaptive SAM) — Definition 3.4.1

Require: L, η, ρ, w_0, T, $\tau > 0$ (minimum weight scale)

for $t = 1$ to T **do**
  Sample mini-batch $\mathcal{B}_t$
  $g_t \leftarrow \nabla_w L_{\mathcal{B}_t}(w_{t-1})$
  $T_w \leftarrow \operatorname{diag}(|w_{t-1,i}| + \tau)_{i=1}^d$ ▷ Adaptive scaling
  $\hat{\varepsilon}_t \leftarrow \rho \cdot T_w^2 g_t / \|T_w g_t\|$ ▷ Scaled perturbation
  $\tilde{g}_t \leftarrow \nabla_w L_{\mathcal{B}_t}(w_{t-1} + \hat{\varepsilon}_t)$
  $w_t \leftarrow w_{t-1} - \eta \tilde{g}_t$
end for
return w_T

C.4 Continual Learning Algorithms

Implementation note for ReDo: it is essential to reset the Adam state (m, v) for reinitialised neurons. Otherwise, the large second moment $\hat{v}_{i,\cdot}$ from before reinitialisation will suppress the learning rate for the reinitialised neuron, preventing it from learning in its new configuration. This is a subtle but important implementation detail not always mentioned in the original paper.

Algorithm 13 m-SAM (Mini-batch SAM) — Definition 3.6.1

Require: L, η, ρ, w_0, T, shards m

for $t = 1$ to T **do**
  Partition mini-batch $\mathcal{B}_t = \mathcal{B}_t^{(1)} \cup \cdots \cup \mathcal{B}_t^{(m)}$
  $\tilde{g}_t \leftarrow 0$
  for $j = 1$ to m **do**
    $g^{(j)} \leftarrow \nabla_w L_{\mathcal{B}_t^{(j)}}(w_{t-1})$
    $\hat{\varepsilon}^{(j)} \leftarrow \rho \cdot g^{(j)} / \left\| g^{(j)} \right\|$
    $\tilde{g}_t \leftarrow \tilde{g}_t + \nabla_w L_{\mathcal{B}_t^{(j)}}(w_{t-1} + \hat{\varepsilon}^{(j)})$
  end for
  $w_t \leftarrow w_{t-1} - \eta \tilde{g}_t / m$
end for
return w_T

Algorithm 14 Elastic Weight Consolidation (EWC) — Section 4.4.2

Require: Tasks $\mathcal{T}_1, \ldots, \mathcal{T}_K$, regularisation strength λ

$w^{(0)} \leftarrow$ random initialisation
for $k = 1$ to K **do**
  Train w on $\mathcal{T}_k$ with loss $L_k(w)$, starting from $w^{(k-1)}$:
  if $k = 1$ **then**
    Standard SGD/Adam on L_k
  else
    Augmented loss: $\hat{L}_k(w) = L_k(w) + \frac{\lambda}{2}(w - w^{(k-1)})^\top F^{(k-1)}(w - w^{(k-1)})$
    Train on $\hat{L}_k$ to convergence $\rightarrow w^{(k)}$
  end if
  Estimate diagonal Fisher at $w^{(k)}$:
  $F_{ii}^{(k)} \leftarrow \frac{1}{n_k} \sum_{j=1}^{n_k} (\nabla_{w_i} \log p_{w^{(k)}}(y_j | x_j))^2$ ▷ Can use Adam's v_t as a free estimate
end for
return $w^{(K)}$

Algorithm 15 Gradient Episodic Memory (GEM) — Section 4.5.2

Require: Tasks $\mathcal{T}_1, \ldots, \mathcal{T}_K$, episodic memory $\mathcal{M}$

$w^{(0)} \leftarrow$ random initialisation, $\mathcal{M} \leftarrow \emptyset$
for $k = 1$ to K **do**
  Sample memory $\mathcal{M}_k \subset \mathcal{T}_k$ (small subset)
  $\mathcal{M} \leftarrow \mathcal{M} \cup \{(\mathcal{M}_k, g_k)\}$ where $g_k = \nabla L_{\mathcal{M}_k}(w^{(k-1)})$
  for each training step on $\mathcal{T}_k$ **do**
    $g \leftarrow \nabla L_{\mathcal{B}}(w)$ ▷ Current task gradient
    if $\langle g, g_j \rangle < 0$ for any $j < k$: ▷ Check for conflict
      Solve QP: $\tilde{g} = \arg\min_v \|v - g\|^2$ s.t. $\langle v, g_j \rangle \geq 0 \; \forall j$
    else: $\tilde{g} \leftarrow g$ ▷ No conflict: use original gradient
    $w \leftarrow w - \eta \tilde{g}$
  end for
  $w^{(k)} \leftarrow w$
end for
return $w^{(K)}$

Algorithm 16 ReDo (Recycling Dormant Neurons) — Section 4.3.2

Require: Network f_w, Adam optimiser state (m, v), reset threshold τ, reset interval Δ

for $t = 1, 2, \ldots$ **do**
  Standard Adam update
  if $t \mod \Delta = 0$ **then** ▷ Periodic plasticity check
    for each layer l, each neuron i **do**
      $s_i \leftarrow \mathbb{E}_x[\|\partial f_w(x)/\partial a_i(x)\|]$ ▷ Dormancy score
      if $s_i < \tau$ **then** ▷ Neuron is dormant
        Reinitialise $w_i^{\text{in}}, w_i^{\text{out}}$ from original initialisation distribution
        Reset Adam state: $m_{i,\cdot} \leftarrow 0$, $v_{i,\cdot} \leftarrow 0$ ▷ Critical: reset momentum for reinitialised neurons
      end if
    end for
  end if
end for

C.5 Diagnostics and Monitoring

Algorithm 17 Hessian Sharpness via Power Iteration

Require: Loss L, weights w, iterations $K = 20$

$v \leftarrow$ random unit vector
for $k = 1$ to K **do**
  $Hv \leftarrow \nabla_w(\langle \nabla_w L(w),\, v \rangle)$ ▷ Hessian-vector product via 2nd-order AD
  $\lambda \leftarrow \|Hv\|$
  $v \leftarrow Hv/\lambda$
end for
return λ ▷ Estimate of $\lambda_{\max}(\nabla^2 L(w))$

Cost: each Hessian-vector product requires one forward pass + two backward passes (or one forward-over-backward). For $d = 10^8$ parameters, this costs $\approx 3\times$ a standard gradient computation. With $K = 20$ iterations, sharpness estimation costs $60\times$ a gradient step — feasible only at validation time, not every step.

Algorithm 18 Effective Rank Monitoring

Require: Weight matrix $W \in \mathbb{R}^{m \times n}$ (per layer)

Compute SVD: $W = U \Sigma V^\top$, singular values $\sigma_1 \geq \cdots \geq \sigma_r > 0$
$\bar{\sigma}_i \leftarrow \sigma_i / \sum_j \sigma_j$ ▷ Normalise
$\text{rank}_{\text{eff}}(W) \leftarrow \exp(-\sum_i \bar{\sigma}_i \log \bar{\sigma}_i)$
return $\text{rank}_{\text{eff}}(W)$, σ_1/σ_r (condition number)

Cost: full SVD costs $O(\min(m,n)^2 \max(m,n))$. For large matrices, use randomised SVD (e.g., `torch.svd_lowrank`) with rank $k = 20$ to estimate the top singular values. The effective rank can then be computed from the top-k singular values with a correction for the remaining mass.

Appendix D: Convex Duality and Minimax Theory

This appendix reviews the convex duality and minimax theory that underlies several key results in the volume: the PAC-Bayes bound (Chapter 3), the SAM minimax formulation (Chapter 3), the GEM quadratic program (Chapter 4), and the Pontryagin optimal control conditions (Chapter 4).

D.1 Fenchel Conjugates

Definition 5.44 (Fenchel conjugate)**.** For a function $f : \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$, the *Fenchel conjugate* is:

$$f^*(y) = \sup_{x \in \mathbb{R}^d} \left[\langle y,\, x \rangle - f(x) \right].$$

Proposition 5.45 (Properties of the conjugate)**.** *(i) f^* is always convex, even if f is not.*
(ii) ***Fenchel–Young inequality****: $\langle x,\, y \rangle \le f(x) + f^*(y)$ for all x, y.*
(iii) ***Biconjugate****: $f^{**} = f$ if and only if f is convex, l.s.c., and proper.*
(iv) For $f(x) = \frac{1}{2}\|x\|^2$: $f^*(y) = \frac{1}{2}\|y\|^2$.
(v) For $f(x) = \|x\|_1$: $f^*(y) = \mathbf{1}[\|y\|_\infty \le 1]$ (indicator of ℓ_∞ ball).
(vi) For $f(x) = \|x\|_\infty$: $f^*(y) = \mathbf{1}[\|y\|_1 \le 1]$ (indicator of ℓ_1 ball).

Example 5.46 (SAM via Fenchel duality)**.** The SAM perturbation problem $\max_{\|\varepsilon\|_2 \le \rho} L(w+\varepsilon)$ can be written as $\max_\varepsilon [L(w+\varepsilon) - \delta_{\mathcal{B}(0,\rho)}(\varepsilon)]$, where $\delta_{\mathcal{B}}$ is the indicator function of the ball. The dual of this problem (in the sense of Fenchel duality applied to the linearised loss) is the problem of finding the gradient of the loss at the perturbed point — exactly the SAM gradient computation (equation 3.5). The duality gap is the approximation error of the first-order perturbation (Proposition 3.4.1).

D.2 Minimax Theorems

Theorem 5.47 (Von Neumann minimax theorem)**.** *Let $X \subset \mathbb{R}^m$ and $Y \subset \mathbb{R}^n$ be non-empty compact convex sets. If $f : X \times Y \to \mathbb{R}$ is convex in x for fixed y and concave in y for fixed x:*

$$\min_{x \in X} \max_{y \in Y} f(x, y) = \max_{y \in Y} \min_{x \in X} f(x, y).$$

Remark 5.48 (SAM is not a true minimax problem). The SAM objective $\min_w \max_{\|\varepsilon\| \le \rho} L(w+\varepsilon)$ looks like a minimax problem, but the inner function $L(w+\varepsilon)$ is not concave in ε in general (for non-convex L). The minimax theorem does not apply, and $\min_w \max_\varepsilon L(w+\varepsilon) \neq \max_\varepsilon \min_w L(w+\varepsilon)$ in general. SAM minimises the maximum perturbation loss, which is a well-posed variational problem even without convexity, but the min-max equality fails. The PAC-Bayes interpretation (Section 3.5) provides the correct theoretical framework.

Theorem 5.49 (Sion's minimax theorem)**.** *Let X be a compact convex subset of a Hausdorff topological vector space, and Y a convex subset of a vector space. If $f : X \times Y \to \mathbb{R}$ is:*

- *quasi-concave and upper semi-continuous in y for each fixed x,*
- *quasi-convex and lower semi-continuous in x for each fixed y,*

then $\min_x \max_y f(x, y) = \max_y \min_x f(x, y)$.

Example 5.50 (Sion's theorem for the GEM QP)**.** The GEM projection (Proposition 4.5.2) solves $\min_v \|v - g\|^2$ subject to $Gv \geq 0$. The Lagrangian dual is $\max_{\mu \geq 0} \min_v [\|v - g\|^2 - \mu^\top G v]$. The inner $\min_v$ gives $v^* = g + G^\top \mu/2$, and the dual is a concave QP in μ. By Sion's theorem (the Lagrangian is convex-concave), strong duality holds: the duality gap is zero, confirming that the dual QP gives the exact primal solution.

D.3 Lagrangian Duality and KKT Conditions

Theorem 5.51 (KKT conditions for constrained optimisation)**.** *For the problem* $\min_x f(x)$ *subject to $g_i(x) \leq 0$, $h_j(x) = 0$: if the problem is convex and Slater's condition holds ($\exists x^*$ with $g_i(x^*) < 0$), then the primal and dual solutions x^*, μ^*, ν^* satisfy:*

$$\nabla f(x^*) + \sum_i \mu_i^* \nabla g_i(x^*) + \sum_j \nu_j^* \nabla h_j(x^*) = 0 \qquad \text{(stationarity)}$$

$$g_i(x^*) \leq 0 \qquad \text{(primal feasibility)}$$

$$\mu_i^* \geq 0 \qquad \text{(dual feasibility)}$$

$$\mu_i^* g_i(x^*) = 0 \qquad \text{(complementary slackness)}$$

and the strong duality holds: $\min_x \max_{\mu \geq 0, \nu} \mathcal{L}(x, \mu, \nu) = \max_{\mu \geq 0, \nu} \min_x \mathcal{L}(x, \mu, \nu)$.

Example 5.52 (EWC as KKT for the sequential task constraint)**.** The continual learning problem (equation 4.4) with constraint $L_{k-1}(w) \leq L_{k-1}(w^{(k-1)}) + \varepsilon$ has the Lagrangian:

$$\mathcal{L}(w, \lambda) = L_k(w) + \lambda(L_{k-1}(w) - L_{k-1}(w^{(k-1)}) - \varepsilon).$$

The KKT stationarity condition is: $\nabla L_k(w^*) + \lambda^* \nabla L_{k-1}(w^*) = 0$. The EWC approximation replaces $\nabla L_{k-1}(w^*)$ with its quadratic expansion around $w^{(k-1)}$: $\nabla L_{k-1}(w^*) \approx F^{(k-1)}(w^* - w^{(k-1)})$. This gives: $\nabla L_k(w^*) + \lambda^* F^{(k-1)}(w^* - w^{(k-1)}) = 0$, the stationarity condition for the EWC loss (equation 4.5) with $\lambda = \lambda^*$. □

D.4 The Pontryagin Maximum Principle: Self-Contained Statement

The Pontryagin Maximum Principle (PMP) is the fundamental tool for optimal control problems, used in Section 4.3.3. We state it self-containedly here.

Theorem 5.53 (Pontryagin Maximum Principle, continuous time)**.** *Consider the optimal control problem:*

$$\begin{aligned} \min_{u(\cdot)} \quad & \int_0^T \ell(w(t), u(t))\, dt + \Phi(w(T)) \\ \text{s.t.} \quad & \dot{w}(t) = f(w(t), u(t)), \quad w(0) = w_0, \\ & u(t) \in \mathcal{U} \quad \textit{(admissible controls)}. \end{aligned}$$

Define the Hamiltonian $\mathcal{H}(w, p, u) = p^\top f(w, u) - \ell(w, u)$, where $p \in \mathbb{R}^d$ is the costate (adjoint) variable. If (w^*, u^*) is an optimal solution, there exists a costate p^* satisfying:

$$\dot{w}^*(t) = \frac{\partial \mathcal{H}}{\partial p}(w^*(t), p^*(t), u^*(t)) = f(w^*(t), u^*(t)) \qquad \text{(state eq.)}$$

$$\dot{p}^*(t) = -\frac{\partial \mathcal{H}}{\partial w}(w^*(t), p^*(t), u^*(t)) \qquad \text{(adjoint eq.)}$$

$$u^*(t) = \arg\max_{u \in \mathcal{U}} \mathcal{H}(w^*(t), p^*(t), u) \qquad \text{(maximality)}$$

$$p^*(T) = -\nabla_w \Phi(w^*(T)). \qquad \text{(transversality)}$$

Remark 5.54 (Application to plasticity control). For the plasticity control problem (Definition 4.3.2), the Hamiltonian is:

$$\mathcal{H}(w, p, u, \lambda) = p^\top(-\nabla L + u) - L(w) - \lambda(p_{\min} - \mathcal{P}(w)),$$

with admissible control $\mathcal{U} = \mathcal{B}(0, \kappa)$. The maximality condition gives $u^* = \kappa p^* / \|p^*\|$ (bang-bang on the ℓ_2 ball). The adjoint equation $\dot{p}^* = \nabla_w L + \lambda^* \nabla_w \mathcal{P}$ accumulates both the loss gradient (driving toward better performance) and the plasticity gradient (driving toward more plastic configurations). This is exactly Proposition 4.3.1.

D.5 The Free Energy and the Variational Principle

The *free energy* of a statistical mechanics system is fundamental to the PAC-Bayes framework and the Gibbs algorithm.

Definition 5.55 (Free energy)**.** For a reference measure P and a function $\phi : \mathcal{W} \to \mathbb{R}$, the *free energy* with inverse temperature β is:

$$F_\beta(\phi) = -\frac{1}{\beta} \log \mathbb{E}_{w \sim P}[e^{\beta \phi(w)}].$$

Theorem 5.56 (Variational representation of free energy)**.**

$$F_\beta(\phi) = \min_{Q \ll P} \left[\mathbb{E}_{w \sim Q}[\phi(w)] + \frac{1}{\beta} \mathrm{KL}(Q \| P) \right],$$

with the minimum attained at the Gibbs posterior $Q^* = P \cdot e^{\beta\phi}/Z_\beta$ (where $Z_\beta = \mathbb{E}_P[e^{\beta\phi}]$ is the partition function).

Proof. By the change-of-measure inequality (Theorem 3.1.1): $\mathbb{E}_Q[\phi] \geq F_\beta(\phi) - \frac{1}{\beta}\mathrm{KL}(Q\|P)$, giving $\mathbb{E}_Q[\phi] + \frac{1}{\beta}\mathrm{KL}(Q\|P) \geq F_\beta(\phi)$ for all Q. Equality holds at Q^*: $\mathrm{KL}(Q^*\|P) = \mathbb{E}_{Q^*}[\log dQ^*/dP] = \mathbb{E}_{Q^*}[\beta\phi - \log Z_\beta] = \beta\mathbb{E}_{Q^*}[\phi] - \log Z_\beta = \beta(\mathbb{E}_{Q^*}[\phi] - F_\beta(\phi))$. □

Remark 5.57 (Connection to PAC-Bayes). The PAC-Bayes bound of Theorem 3.2.1 with $\beta = n$ (inverse sample size) is exactly the statement that the free energy $F_n(-L_{\text{pop}})$ is bounded below by $-L_{\text{train}}(Q) - \frac{1}{n}\mathrm{KL}(Q\|P) -$ statistical error. The Gibbs algorithm minimises the free energy, which is the tightest PAC-Bayes bound. SAM minimises an upper bound on the free energy (the worst-case perturbation loss), which is tractable but not optimal.

Appendix E: Hints and Selected Solutions

This appendix provides hints and complete solutions for selected exercises from the main chapters. Exercises marked **[S]** have complete solutions here; exercises marked **[H]** have hints only.

Chapter 1 Solutions

Exercise 1.1 [S]: Morse inequality on the torus. The height function $f(x, y) = \cos(2\pi x) + 2\cos(2\pi y)$ on T^2 has critical points where $\partial_x f = \partial_y f = 0$: $-2\pi \sin(2\pi x) = 0 \Rightarrow x \in \{0, 1/2\}$; $-4\pi \sin(2\pi y) = 0 \Rightarrow y \in \{0, 1/2\}$.

Four critical points: $(0,0), (0,1/2), (1/2,0), (1/2,1/2)$.

Hessian at each point: $H = \begin{pmatrix} -4\pi^2 \cos(2\pi x) & 0 \\ 0 & -8\pi^2 \cos(2\pi y) \end{pmatrix}$.

At $(0,0)$: $H = \mathrm{diag}(-4\pi^2, -8\pi^2)$ — both negative — **local maximum** (index 2). At $(0,1/2)$: $H = \mathrm{diag}(-4\pi^2, +8\pi^2)$ — mixed signs — **index-1 saddle**. At $(1/2,0)$: $H = \mathrm{diag}(+4\pi^2, -8\pi^2)$ — mixed signs — **index-1 saddle**. At $(1/2,1/2)$: $H = \mathrm{diag}(+4\pi^2, +8\pi^2)$ — both positive — **local minimum** (index 0).

Count: $c_0 = 1, c_1 = 2, c_2 = 1$. Alternating sum: $1 - 2 + 1 = 0 = \chi(T^2)$. ✓

Exercise 1.2(b) [S]: Index computation via semicircle. For $H = M - \mu I$ with $\mu = 1$ ($d = 100$): $p_-(\mu) = \int_{-\infty}^{0} \rho_{\mathrm{sc}}(\lambda + \mu)\, d\lambda = \int_{-\infty}^{-\mu} \rho_{\mathrm{sc}}(\lambda)\, d\lambda$.

For $\mu = 1$: $p_-(1) = \int_{-2}^{-1} \frac{1}{2\pi}\sqrt{4 - \lambda^2}\, d\lambda$.

Using the substitution $\lambda = 2\sin\theta$: $p_-(1) = \frac{1}{2\pi}\int_{-\pi/2}^{-\pi/6} 2\cos\theta \cdot 2\cos\theta\, d\theta = \frac{2}{\pi}\int_{-\pi/2}^{-\pi/6} \cos^2\theta\, d\theta$. $= \frac{2}{\pi}\left[\frac{\theta}{2} + \frac{\sin 2\theta}{4}\right]_{-\pi/2}^{-\pi/6} = \frac{2}{\pi}\left[(-\frac{\pi}{12} + \frac{\sin(-\pi/3)}{4}) - (-\frac{\pi}{4} + 0)\right] = \frac{2}{\pi}\left[-\frac{\pi}{12} - \frac{\sqrt{3}}{8} + \frac{\pi}{4}\right] = \frac{2}{\pi}\left[\frac{\pi}{6} - \frac{\sqrt{3}}{8}\right]$ $= \frac{1}{3} - \frac{\sqrt{3}}{4\pi} \approx 0.333 - 0.138 \approx 0.195$.

Expected index at $d = 100$: $\approx 100 \times 0.195 = 19.5 \approx 20$ negative eigenvalues.

Exercise 1.4 [H]: Condition number and Adam advantage. Hint: Compute the eigenvalues of $\nabla^2 L|_{W^*}$ using the Kronecker product formula. Show that the condition number $\kappa \approx (\sigma_1(W^*)/\sigma_2(W^*))^2 \approx 47.5$. Then compute Adam's effective step sizes in each singular direction and show they are approximately equal (condition-number-free), giving convergence rate $\approx (1 - \eta)^t$ in all directions.

Exercise 1.5 [S]: Batch size for SGD escape. From Proposition 1.5.2, the escape condition requires $r \leq O(1/\sqrt{B})$ where r is the effective noise radius. The PGD requirement is $r = O(\delta\gamma^2/(\rho\ell d))$. Setting these equal: $B \leq O(\rho^2\ell^2 d^2/(\delta^2\gamma^4))$. For $\gamma = 0.1$ (smallest negative eigenvalue), $\rho = 1$, $\ell = 10$, $d = 100$, $\delta = 0.05$: $B \leq O(1 \times 100 \times 10000/(0.0025 \times 0.0001)) = O(4 \times 10^{10})$. This bound is not tight in practice — the noise from mini-batching is sufficient for much larger batch sizes. The key: for $B = 32$ (typical small batch), the noise is $\sigma_{\min}/\sqrt{32}$, and we need $\sigma_{\min}/\sqrt{32} \geq r_{\mathrm{PGD}}$. For the given problem, $\sigma_{\min} \approx 0.1$ (typical gradient variance), giving $r_{\mathrm{eff}} \approx 0.018$, which exceeds $r_{\mathrm{PGD}} \approx 10^{-5}$ by a large margin.

Chapter 2 Solutions

Exercise 2.1 [S]: Adam on the quadratic loss. For constant $g_t = g$ and $\beta_1 = 0$: $m_t = g$, so $\hat{m}_t = g(1-\beta_1^t)^{-1} \cdot (1-\beta_1) \cdot g = g$. For $g_t = g > 0$ constant, the update is $w_{t+1} = w_t - \eta g/(\sqrt{\hat{v}_t}+\varepsilon) \approx w_t - \eta\,\mathrm{sgn}(g) = w_t - \eta$. On $L(w) = \frac{1}{2}(w-w^*)^2$: $g_t = w_t - w^* > 0$ (for $w_0 > w^*$). Adam takes steps of constant size η: $w_t = w_0 - \eta t$ until $w_t = w^*$. Convergence time: $T = (w_0 - w^*)/\eta$. This is *finite-time convergence*, unlike GD which decays exponentially. The sign gradient descent (Adam with $\beta_2 \to 0$) has *better* finite-time convergence on the quadratic than GD for this reason.

Exercise 2.3 [H]: Counter-example implementation. Hint: Implement the loss sequence with $f_t(x) = Cx\mathbf{1}[t \mod 3 = 0] - x\mathbf{1}[t \mod 3 \neq 0]$. The divergence should be clear for $C = 3$: plot w_t and verify it is monotonically increasing. For AMSGrad: the monotone $\hat{v}_t$ prevents the effective learning rate from inflating, so the iterate converges. The transition between Adam (divergent) and AMSGrad (convergent) should be observable at $C = 2+\varepsilon$ for small $\varepsilon > 0$.

Exercise 2.5 [S]: $\beta_1 < \sqrt{\beta_2}$ condition. (a) $\beta_1 = 0.9$, $\beta_2 = 0.999$: $\sqrt{0.999} \approx 0.9995 > 0.9$. **Satisfied**. ✓ (b) $\beta_1 = 0.95$, $\beta_2 = 0.98$: $\sqrt{0.98} \approx 0.9899 > 0.95$. **Satisfied**. ✓ (c) $\beta_1 = 0.98$, $\beta_2 = 0.98$: $\sqrt{0.98} \approx 0.9899 > 0.98$. **Satisfied** (barely). ✓ All three satisfy the condition. The bound deteriorates for (c) since $\beta_1 \approx \sqrt{\beta_2}$.

Chapter 3 Solutions

Exercise 3.1 [S]: Change-of-measure inequality proof. For any two distributions Q, P and function ϕ:

$$\mathbb{E}_{w\sim Q}[\phi(w)] = \mathbb{E}_{w\sim Q}\left[\phi(w) - \log \frac{dQ}{dP}(w)\right] + \mathrm{KL}(Q\|P).$$

By Jensen's inequality (applied to the concave function log):

$$\mathbb{E}_{w\sim Q}\left[\phi(w) - \log \frac{dQ}{dP}(w)\right] = \mathbb{E}_{w\sim Q}\left[\log \frac{e^{\phi(w)}dP(w)}{dQ(w)}\right] \leq \log \mathbb{E}_{w\sim Q}\left[\frac{e^{\phi(w)}dP(w)}{dQ(w)}\right] = \log \mathbb{E}_{w\sim P}[e^{\phi(w)}].$$

Combining: $\mathbb{E}_Q[\phi] \leq \mathrm{KL}(Q\|P) + \log \mathbb{E}_P[e^{\phi}]$. □

Exercise 3.2 [S]: PAC-Bayes bound numerics. $n = 10000$, $\delta = 0.01$, KL $= 5$: $L_{\text{pop}} \leq L_{\text{train}} + \sqrt{\frac{5+\log(10000/0.01)}{2\times 9999}} = L_{\text{train}} + \sqrt{\frac{5+13.8}{19998}} = L_{\text{train}} + \sqrt{9.4\times 10^{-4}} = L_{\text{train}} + 0.031$. The trivial bound (from $\ell \in [0,1]$) is $L_{\text{pop}} \leq 1$. The PAC-Bayes bound is tighter than the trivial bound when $L_{\text{train}} + 0.031 < 1$, i.e., $L_{\text{train}} < 0.97$. For near-zero training loss, the PAC-Bayes bound gives a test loss bound of ≈ 0.031 — informative for a 10000-sample dataset.

Exercise 3.4 [H]: SAM bound under reparametrisation. Hint: Compute $\|\tilde{w}\|_2^2 = \alpha^2\|w_{1:k}\|^2 + \|w_{k+1:d}\|^2$ and show it grows as $O(\alpha^2)$. Compute $\max_{\|\varepsilon\|\leq\rho}[L(\tilde{w}+\varepsilon) - L(\tilde{w})]$ using the first-order approximation and show it decreases as $O(1/\alpha)$ (the gradient in the rescaled coordinates is $O(1/\alpha)$ smaller). Show the product (sharpness term × complexity term) is approximately constant.

Chapter 4 Solutions

Exercise 4.1 [S]: Pontryagin for the quadratic. For $L(w) = \frac{1}{2}\|w\|^2$, $\mathcal{P}(w) = e^{-\|w\|^2}$, $p_{\min} = 0.5$. The Hamiltonian is $\mathcal{H}(w,p,u,\lambda) = p^\top(-w+u) - \frac{1}{2}\|w\|^2 - \lambda(0.5 - e^{-\|w\|^2})$. State

equation: $\dot{w} = -w + u$. Adjoint equation: $\dot{p} = w - \lambda \cdot (-2we^{-\|w\|^2}) = w(1 + 2\lambda e^{-\|w\|^2})$. Control law: $u^* = \kappa p / \|p\|$ (bang-bang).

Constraint $\mathcal{P}(w) \geq 0.5$: active when $e^{-\|w\|^2} = 0.5$, i.e., $\|w\|^2 = \log 2 \approx 0.693$. So t^* is when $\|w(t)\|^2 = \log 2$ (the constraint activates as the iterate moves away from 0).

Exercise 4.2 [S]: EWC minimiser at $\lambda = 5$. From Example 4.6.2: $w^*_{\text{EWC}} = \frac{e_2 + \lambda e_1}{1+\lambda} = \frac{(0,1,0)+5(1,0,0)}{6} = \frac{(5,1,0)}{6} = (5/6, 1/6, 0)$. $L_1(w^*) = \frac{1}{2}\|(5/6, 1/6, 0) - (1,0,0)\|^2 = \frac{1}{2}((-1/6)^2 + (1/6)^2) = \frac{1}{2} \times 2/36 = 1/36 \approx 0.028$. $L_2(w^*) = \frac{1}{2}\|(5/6, 1/6, 0) - (0,1,0)\|^2 = \frac{1}{2}((5/6)^2 + (-5/6)^2) = \frac{1}{2} \times 50/36 = 25/36 \approx 0.694$. Sum: $\approx 0.028 + 0.694 = 0.722$. Minimum sum: $\min_w[L_1 + L_2] = \min_w \frac{1}{2}[\|w - e_1\|^2 + \|w - e_2\|^2]$ achieved at $w = (e_1 + e_2)/2 = (1/2, 1/2, 0)$, giving sum $= 2 \times \frac{1}{2} \times \frac{1}{2} = 0.5$. So EWC with $\lambda = 5$ achieves 0.722 vs. optimal 0.500 — the regularisation prevents reaching the global optimum of the combined loss.

Chapter 5 Solutions

Exercise 5.1 [S]: Flat-and-plastic construction. Let $d = 4$, $W = I_2 \in \mathbb{R}^{2\times 2}$ (identity matrix as the weight matrix of the single layer), with loss $L(W) = \frac{\varepsilon}{2}\|W - I\|^2$ for $\varepsilon = 0.01$ (very flat).

- Sharpness: $\lambda_{\max}(\nabla^2 L(W^*)) = \varepsilon = 0.01$ — flat. ✓
- Effective rank: $\sigma_1 = \sigma_2 = 1$ for $W^* = I$, so $\text{rank}_{\text{eff}}(I) = \exp(-2 \times \frac{1}{2} \log \frac{1}{2}) = \exp(\log 2) = 2$. Maximum rank (both singular values equal). ✓
- Dead neurons: for $W = I$ and ReLU, $z_i = e_i^\top x$ (the i-th coordinate of x). For $x \sim \mathcal{N}(0, I)$: $\mathbb{P}[z_i \leq 0] = 0.5$, so $\phi_{\text{dead}} = 0.5$ (half the neurons are dead for any given input, but none are permanently dead). $\mathcal{P}(W^*) = 1 - \phi_{\text{dead}} = 0.5$ for $\alpha = 1$. ✓ (Flat and moderately plastic.)

Exercise 5.3 [H]: Hessian through four chapters. Hint: Use the two-layer network from Section 1.8 with the explicit values computed there. (a) At the saddle $(W_1 = 0, W_2 = 0)$: $H = \begin{pmatrix} 0 & C \\ C^\top & 0 \end{pmatrix}$ with $C = \frac{1}{n}\partial^2 L/(\partial W_2 \partial W_1)$. Compute C using the Khatri–Rao product of the data matrices. The index is 4 (half the 8×8 Hessian eigenvalues are negative). (b) Edge of stability for Adam: $\ell_i^{\text{eff},*} = 2\hat{v}_i^{1/2}/\eta$. At the global minimum, $\hat{v}_i \approx F_{ii} \approx \lambda_i^2(H)\Gamma_i$ (stationary distribution variance). Compute numerically. (c) SAM perturbation: $\hat{\varepsilon} = 0.1 \times \nabla L / \|\nabla L\|$ at the halfway point. (d) Fisher diagonal: $F_{ii} = \hat{v}_{\infty,i}$ at the global minimum (Adam second moment).

Cross-Chapter Solutions

Problem Cross-1 [S]: Hessian through all four chapters (complete solution).

We work through the two-layer linear network $L(W_1, W_2) = \frac{1}{2n}\|W_2 W_1 X - Y\|_F^2$ with $d_0 = d_2 = k = 2$, $n = 4$, $X = \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{pmatrix}$, $Y = \begin{pmatrix} 2 & 1 & 2 & 1 \\ 1 & 3 & 1 & 3 \end{pmatrix}$.

(a) Chapter 1 — Index at the saddle. At $(W_1, W_2) = (0, 0)$ all parameters are zero. The Hessian of L with respect to the 8-dimensional parameter vector $\theta = (\text{vec}(W_1)^\top, \text{vec}(W_2)^\top)^\top$ has the block structure:

$$H|_0 = \frac{1}{n}\begin{pmatrix} 0 & B \\ B^\top & 0 \end{pmatrix},$$

where $B \in \mathbb{R}^{4\times 4}$ captures the cross-second-derivatives $\partial^2 L/(\partial W_2 \partial W_1)$.

By the block structure, the eigenvalues of $H|_0$ are $\pm\sigma_i(B/n)$ for $i = 1, \ldots, 4$. Since B is generically full rank (for the given data), there are 4 positive and 4 negative eigenvalues: **index = 4**. This confirms Theorem 1.13: the origin is a strict saddle with index $= k^2 = 4$ (where $k = 2$ is the hidden dimension).

(b) Chapter 2 — Adam edge of stability. At the global minimum $W^* = \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix}$ (computed in Section 1.8), the Hessian of L restricted to variations of (W_1, W_2) around any factorisation $W_2^* W_1^* = W^*$ has eigenvalues proportional to $\sigma_i(W^*)^2/n$.

Singular values of W^*: $\sigma_1 \approx 3.30$, $\sigma_2 \approx 0.61$ (from $\mathrm{tr}(W^{*\top} W^*) = 4 + 1 + 1 + 9 = 15$ and $\det(W^{*\top} W^*) = \det(W^*)^2 = (6-1)^2 = 25$, giving $\sigma_1^2 + \sigma_2^2 = 15$, $\sigma_1^2 \sigma_2^2 = 25$: $\sigma_1^2 \approx 10.9$, $\sigma_2^2 \approx 4.1$... wait, let us recompute. $W^{*\top} W^* = \begin{pmatrix} 4+1 & 2+3 \\ 2+3 & 1+9 \end{pmatrix} = \begin{pmatrix} 5 & 5 \\ 5 & 10 \end{pmatrix}$. Eigenvalues: $\lambda = \frac{15 \pm \sqrt{225-200}}{2} = \frac{15 \pm 5}{2}$, giving $\lambda_1 = 10$, $\lambda_2 = 5$. So $\sigma_1 = \sqrt{10} \approx 3.16$, $\sigma_2 = \sqrt{5} \approx 2.24$.

The largest Hessian eigenvalue at W^*: $\lambda_{\max}(H|_{W^*}) \approx 2\sigma_1^2/n = 2 \times 10/4 = 5$. Adam's edge of stability with $\eta = 10^{-3}$: at stationarity, $\hat{v}_{\max} \approx F_{\max} \approx \lambda_{\max}^2(H)\Gamma_{\max}$. Using $\Gamma_{\max} \approx \eta\sigma_g^2/(2\lambda_{\max}) \approx 10^{-3} \times 1/(2 \times 5) = 10^{-4}$: $\ell^{\mathrm{eff},*} = 2\sqrt{\hat{v}_{\max}}/\eta \approx 2\sqrt{5 \times 10^{-4}}/10^{-3} \approx 2 \times 0.022/10^{-3} \approx 45$. Much larger than $\lambda_{\max} = 5$: Adam is stable with large margin.

(c) Chapter 3 — SAM perturbation. At the midpoint $(W_1, W_2) = (0.5W_1^*, 0.5W_2^*)$ with $W_2 W_1 = 0.25W^*$: $L(0.5W) = \frac{1}{2n}\|0.25W^*X - Y\|_F^2$. $\nabla_{W_2} L = \frac{1}{n}(0.25W^*X - Y)X^\top W_1^\top = \frac{1}{4n}(0.25W^* - YX^\dagger)XX^\top W_1^\top$. For the SAM perturbation with $\rho = 0.1$: $\hat{\varepsilon} = 0.1 \times \nabla L / \|\nabla L\|_F$. The gradient at the midpoint is $\frac{3}{4}\|\nabla L|_{W^*}\|_F$ times the full gradient direction (approximately, since the loss is quadratic). The perturbation points toward the global minimum.

(d) Chapter 4 — EWC Fisher diagonal. At the global minimum W^* for a Gaussian model $p_{W^*}(y|x) = \mathcal{N}(W^*x, \sigma^2 I)$: $F_{ij,ij} = \frac{1}{\sigma^4}\mathbb{E}_x[(W^*x)_i^2 x_j^2]$. For $x \sim \mathcal{N}(0, I)$: $\mathbb{E}[(W^*x)_i^2 x_j^2] = (W^*W^{*\top})_{ii}\delta_{jj} = \sigma_1^2 + \sigma_2^2 = 15$ (for $i = 1, 2$, using $\mathrm{tr}(W^{*\top}W^*) = 15$). Diagonal Fisher: $\hat{F}_{ij,ij} \approx 15/\sigma^4$ (uniform across entries of W^*). For $\sigma^2 = 1$: $F_{ii} \approx 15$ for all parameters. The EWC penalty would penalise all weight changes equally.

Cross-chapter insight: The same object — $\sigma_1^2 + \sigma_2^2 = \mathrm{tr}(W^{*\top}W^*) = 15$ — appears in: (a) the index calculation (through the singular values of B), (b) the Hessian eigenvalues at the minimum (proportional to σ_i^2), (c) the SAM gradient magnitude at the midpoint, and (d) the diagonal Fisher at the minimum. This is the Hessian-as-unifying-object of Chapter 5 in concrete form.

Notes on the Appendices

Appendix A: Random Matrix Theory

The random matrix theory summarised in Appendix A draws on a rich mathematical tradition. The Gaussian Orthogonal Ensemble (GOE) was introduced by Wigner (1955) in the context of nuclear physics; his semicircle law (Theorem A.1) has since become one of the central results of probability theory. The definitive mathematical treatment is Anderson, Guionnet, and Zeitouni (2010), *An Introduction to Random Matrices* (Cambridge University Press), which covers the method of moments proof (sketched in Section 1.3.1), the Stieltjes transform approach, and the universality results that extend the semicircle law beyond the Gaussian case.

The Marchenko–Pastur law for sample covariance matrices was established by Marchenko and Pastur (1967) and later given a modern proof via the Stieltjes transform by Silverstein and Bai (1995). The BBP (Baik–Ben Arous–Péché) phase transition (Theorem A.2) was proved in Baik, Ben Arous, and Péché (2005, *Annals of Probability*) and extended to the real (GOE) case by Bai and Yao (2012).

Free probability theory (Section A.3) was developed by Voiculescu in the 1980s as an analogy of classical probability theory for non-commutative random variables. Its application to random matrices was established in Voiculescu, Dykema, and Nica (1992), *Free Random Variables* (AMS). The connection to deep learning Hessians is developed in Fan and Montanari (2019) and Louart, Liao, and Couillet (2018).

The Tracy–Widom distribution (Section A.4) was introduced in Tracy and Widom (1994, *Communications in Mathematical Physics*) for the GUE (complex Hermitian ensemble) and extended to the GOE by Forrester and Witte (2000). Its application to the edge of stability (Remark A.3) is qualitative; a rigorous connection between the Tracy–Widom fluctuations and the discrete-time edge of stability phenomenon requires understanding the interaction between the nonlinear optimiser dynamics and the spectrum fluctuations.

Appendix B: Notation

The notation in this volume follows largely standard conventions in optimisation and machine learning, with some choices motivated by clarity for the specific proofs. The Hessian is always denoted ∇^2 (not H which is reserved for Hessian matrices) and the gradient ∇ (not ∇, though we use ∇ in the text for readability). The inner product $\langle u, v \rangle = u^\top v$ for column vectors; for matrices, $\langle A, B \rangle = \operatorname{tr}(A^\top B)$.

The notation for probability measures follows Villani (2008) for optimal transport, and the Wasserstein gradient flow notation follows Ambrosio, Gigli, and Savaré (2008), *Gradient Flows in Metric Spaces and in the Space of Probability Measures* (Birkhäuser).

Appendix C: Algorithms

The pseudocode in Appendix C follows the conventions of Shalev-Shwartz and Ben-David (2014), *Understanding Machine Learning* (Cambridge University Press), with adaptations for the matrix-valued updates of Muon and the particle-flow updates of SVGD.

The Newton–Schulz iteration for the polar factor (used in the Muon update, Section C.2) converges quadratically when $\sigma_{\max}(A)/\|A\|_F < 1$. For random matrices, this condition is satisfied with probability 1 as $d \to \infty$ (since $\sigma_{\max}(A)/\|A\|_F \leq 1$ with equality only for rank-1 matrices). A proof of convergence for the finite-dimensional case appears in Higham (2008), *Functions of Matrices: Theory and Computation* (SIAM), Chapter 8.

Appendix D: Convex Duality

The convex duality theory of Appendix D follows Rockafellar (1970), *Convex Analysis* (Princeton University Press), for the Fenchel conjugate, and Borwein and Lewis (2006), *Convex Analysis and Nonlinear Optimization* (Springer), for the minimax theorems.

The free energy variational principle (Section D.5) connects to the large deviation theory of Varadhan (1966) and the entropy regularisation of online learning (Hazan, 2016, *Introduction to Online Convex Optimization*). The connection to PAC-Bayes was made explicit by Catoni (2007), who showed that the PAC-Bayes bound is the statistical analogue of the free energy.

The Pontryagin Maximum Principle (Section D.4) is proved in the original monograph by Pontryagin, Boltyanskii, Gamkrelidze, and Mishchenko (1962) and given a modern treatment with convex analysis in Luenberger (1969), *Optimization by Vector Space Methods* (Wiley). The application to the plasticity control problem (Section 4.3.3) is new.

Appendix E: Selected Solutions

The solutions in Appendix E are provided for pedagogical purposes and represent one correct approach; many exercises admit multiple valid proofs. For computational exercises, the numerical values are computed with exact arithmetic where possible and floating-point approximations (to 3–4 significant figures) where not.

The exercises in this volume are graded as follows:

- **[C] Computational**: require numerical computation or implementation. Expected time: 1–3 hours.
- **[A] Analytical**: require mathematical proof. Expected time: 2–6 hours.
- **[R] Research**: open-ended problems requiring literature review and original contribution. Expected time: days to weeks.

All exercises marked [S] (solution provided) or [H] (hint provided) in Appendix E are from the [C] and [A] categories. The [R] problems in the Extended Problem Sets (Chapter 6) have no complete solutions — they are genuine open problems at the time of writing.

A Note on Conventions and Terminology

Several terms in this volume admit multiple conventions in the literature:

- **"Sharpness"**: used for both $\lambda_{\max}(\nabla^2 L)$ (spectral sharpness, used in Chapter 2 for the edge of stability) and $\max_{\|\varepsilon\| \leq \rho} L(w+\varepsilon) - L(w)$ (perturbation sharpness, used in Chapter 3 for SAM). We distinguish these explicitly.

- **"Flat minimum"**: a minimum with small sharpness. The exact threshold ("how small is flat?") depends on context: in Chapter 3, $\lambda_{\max}(H) \leq C/\rho^2$ for some constant C; in Chapter 2, $\lambda_{\max}(H) \leq 2/\eta$ (edge of stability condition).
- **"Plasticity"**: used for the network's ability to learn new tasks (Chapter 4). Not to be confused with "synaptic plasticity" in neuroscience, which refers to the ability of individual synapses to change strength (a lower-level concept).
- **"Natural gradient"**: the preconditioned gradient $F^{-1}\nabla L$. In some sources, "natural gradient" refers specifically to the Amari (1998) formulation for exponential families; in others, it refers to any Riemannian gradient. We use it in the former sense throughout.

We hope these clarifications help readers navigate the broader literature, where the same result may appear under different names and the same name may refer to different results.